Ligand-binding domain of the ultraspiracle (USP) protein

The invention relates to the spatial structure of the ligand-binding domain of the ultraspiracle protein, to the use of this structure for generating protein models of this protein in various conformations and of related proteins, and to methods of finding ligands of the ultraspriracle protein and of related proteins.

The ultraspiracle protein (termed USP hereinbelow) is the insect orthologue of the vertebrate retinoid X receptor (RXR). Like RXR, it belongs to the family of the nuclear receptors (NR). These nuclear receptors are located in the interior of the cell. They bind to responsive elements on the DNA as homo- or heterodimers and regulate the expression of genes. In order to be active they must bind specific small, frequently hydrophobic, ligands (for example steroids, retinoids, vitamin D). Nuclear receptors have a modular structure with functional domains for transactivation, DNA-binding and ligand-binding. While the DNA-binding domain of the nuclear receptors is highly conserved, the ligand-binding domains only show moderate homologies among each other. The spatial structures of various ligand-binding domains have already been determined (summary in 2) and allow an insight into the mechanism on which the activation is based, which comprises pronounced changes in the conformation of the ligand-binding domains. The binding of agonists leads to activation owing to the displacement of bound corepressors and the binding of coactivators, while the binding of antagonists prevents the interaction with the coactivator.

No spatial structures are available yet of insect nuclear receptors. In insects, for example the development from the larva to the adult insect is governed by nuclear receptors and involves the steroid hormone ecdysone and the isoprenoid juvenile hormone (3, 4, 5, 6). The ecdysone receptor, a nuclear receptor composed of two different subunits, EcR and USP, plays a key role in this process (7, 8, 9). It has been

known for a long time that the hormone ecdysone (in its active form 20-hydroxy-ecdysone) acts as ligand for the EcR subunit.

The ecdysone receptor constitutes an important insecticide target. If it is activated outside the windows in the period provided for insect development, this leads to severe damage or even to the death of the insects. The insecticidal action of ecdysone agonists is based on this mechanism (10, 11). Non-steroidal ligands of the EcR sub-unit which act specifically on Lepidoptera are already being used commercially as in-secticides (12).

USP is an orphan receptor for which no ligand is known as yet. While various authors have assumed that USP constitutes a receptor for juvenile hormones, this has never been proven by actual experiments (9). Indeed, it has been assumed that USP has no ligand at all, as this is described for some other nuclear receptors known from animals.

It was therefore an object of the present invention to provide the spatial structure of the ligand-binding domain (termed LBD hereinbelow) of the USP and to describe the possible ligand-binding pocket.

The object was achieved by providing a USP-LBD in crystalline form and by successfully carrying out the X-ray structure analysis of the crystals thus obtained.

The crystalline LBD according to the invention is preferably an LBD of the Heliothis virescens USP. The LBD according to the invention especially preferably has an amino acid sequence shown in SEQ ID NO: 1.

The subject-matter of the present invention is also a crystalline complex of a USP-LBD with a ligand.

The LBD according to the invention preferably has the structure coordinates defined in Table 1. The three-dimensional structure was solved and fully refined with the aid of protein crystals which are accessible to X-ray structure analysis at high resolution by means of molecular replacement. Subject-matter of the present invention is thus also the three-dimensional structure of the USP-LBD which can be determined with the aid of these structure coordinates.

A ligand-binding pocket, into which – like in the case of the other known structures of nuclear receptors – the ligands bind, has been identified in the three-dimensional structure according to the invention of the USP-LBD described herein. This is the first actual confirmation for the fact that USP has a functional ligand-binding pocket.

Subject-matter of the present invention is furthermore a USP-LBD comprising a ligand-binding pocket which is defined by the amino acids LEU230, VAL238, PRO239, PHE242, LEU249, LEU291, ILE294, MET323, LEU331, GLN338, ALA339, VAL341, PHE345, SER431, HIS434, LEU435, PHE438 and LEU440 as shown in SEQ ID NO: 2 and Table 1.

Subject-matter of the present invention is furthermore a USP-LBD comprising a ligand-binding pocket defined by the amino acids LEU230, VAL238, PRO239, PHE242, PRO245, VAL246, LEU249, CYS250, GLY253, ASN287, LEU290, LEU291, ILE294, MET323, LEU325, LEU331, SER335, ALA336, GLN338, ALA339, VAL341, ILE344, PHE345, VAL348, SER431, HIS434, LEU435, PHE438 and LEU440 as shown in SEQ ID NO: 2 and Table 1.

Subject-matter of the present invention is furthermore a USP-LBD comprising a ligand-binding pocket which is defined by the above-described amino acids and in which one or more of these amino acids are mutated. These are preferably conservative mutations, where an amino acid is exchanged for an amino acid with similar physical properties.

Such conservative substitutions encompass variations in which an amino acid is replaced by another amino acid from amongst the following group:

1. Small aliphatic residues, nonpolar residues or residues of little polarity: Ala, Ser, Thr, Pro and Gly;
2. Polar, negatively charged residues and their amides: Asp, Asn, Glu and Gln;
3. Polar, positively charged residues: His, Arg and Lys;
4. Large aliphatic nonpolar residues: Met, Leu, Ile, Val and Cys; and
5. Aromatic residues: Phe, Tyr and Trp.

Preferred conservative substitutions can be seen from the following list:

Original residue	Substitution
Ala	Gly, Ser
Arg	Lys
Asn	Gln, His
Asp	Glu
Cys	Ser
Gln	Asn
Glu	Asp
Gly	Ala, Pro
His	Asn, Gln
Ile	Leu, Val
Leu	Ile, Val
Lys	Arg, Gln, His
Met	Leu, Tyr, Ile
Phe	Met, Leu, Tyr
Ser	Thr
Thr	Ser
Trp	Tyr, Phe
Tyr	Trp, Phe
Val	Ile, Leu

The three-dimensional structure described herein of a USP-LBD is of great importance for the search for ligands with practical application. Such ligands can be used, for example, as insecticides with a novel mechanism of action. The ecdysone/juvenile hormone-governed development is only found in invertebrates and not in vertebrates; thus, it constitutes an insecticidal mechanism which is safe for the user and the environment.

Using the three-dimensional structure according to the invention of the USP-LBD, databases which contain the structures of a large number of compounds can be screened

with the aid of established, automated computer protocols (virtual screening). Algorithms such as FLEXX (13) or GOLD (14) are examples which can be used for virtual screening. With this procedure, compounds can be identified whose three-dimensional structure makes it possible to enter the binding pocket and to bind there, for example by forming hydrogen bonds, by hydrophobic interaction, by electrostatic interactions, by van-der-Waals interactions or by dipole interactions. The compounds identified thus can be synthesized and then used as, for example, insecticides or as effectors in expression systems (gene switch) based on the USP.

Another application of the three-dimensional structure according to the invention of the USP-LBD is the generation of new ligands. To this end, structural formulae for new ligands are generated on the computer using this structure and with the aid of established *de-novo* design programs, and these new ligands can enter the binding pocket, where they can bind, for example by forming hydrogen bonds, by hydrophobic interaction, by electrostatic interactions, by van-der-Waals interactions or by dipole interactions. Examples of *de-novo* design programs which are possible are LUDI (15), LEGEND (16) or GROW (17). Compounds generated thus can be synthesized and then also be used as, for example, insecticides or as effectors in expression systems (gene switch) based on the USP.

The three-dimensional structure according to the invention of the USP-LBD also makes it possible to predict the three-dimensional structure of a USP-LBD from other organisms by means of modelling methods. Such protein models can be used in the same manner as the three-dimensional structure solved herein. Comparison of the differences in the amino acid sequences makes it possible to predict differences in the ligand-binding pockets of various organisms. This is of use when specific ligands are searched for for specific organisms, or, conversely, when it is precisely unspecific ligands that are searched for. In addition, the three-dimensional structure according to the invention can be used for establishing protein models of other nuclear receptors with related sequences.

The present invention encompasses in particular the following subject matters and methods:

A computer-readable data storage medium comprising a data storage material on which the structure coordinates of an LBD according to the present invention are stored.

A computer-readable data storage medium in a form which makes it possible to generate a three-dimensional image of an LBD according to the present invention on a computer screen.

A method of generating protein models of USP-LBDs, characterized by the computer-aided generation of a three-dimensional image of an LBD according to the present invention.

A method of generating protein models of USP-LBDs in an agonistic conformation, characterized by the computer-aided generation of a three-dimensional image of an LBD according to the present invention in an agonistic conformation.

A method of generating protein models of nuclear receptors which have homologies with USP-LBDs, characterized by the computer-aided generation of a three-dimensional image of an LBD according to the present invention with a mutated amino acid sequence.

A method for generating protein models of nuclear receptors which have homologies with USP-LBDs in an agonistic conformation, characterized by the computer-aided generation of a three-dimensional image of an LBD according to the present invention with a mutated amino acid sequence in an agonistic conformation.

A method of finding USP ligands, characterized by the following steps:

(a) the computer-aided generation of a three-dimensional image of an LBD according to the present invention, and

(b) the computer-aided (virtual) screening of databases which contain structural data of chemical compounds for those structures which are capable of undergoing specific interactions with an LBD according to the present invention.

A method of finding USP ligands, characterized by the following steps:

(a) the computer-aided generation of a three-dimensional image of an LBD according to the present invention, and

(b) the computer-aided modelling of chemical compounds with structures which are capable of undergoing specific interactions with an LBD according to the present invention.

A method of finding USP-LBD ligands in an agonistic conformation, characterized by the following steps:

(a) the computer-aided generation of a three-dimensional image of an LBD according to the present invention in an agonistic conformation, and

(b) the computer-aided (virtual) screening of databases which contain structural data of chemical compounds for those structures which are capable of undergoing specific interactions with an LBD in an agonistic conformation.

A method of finding USP-LBD ligands in an agonistic conformation, characterized by the following steps:

(a) the computer-aided generation of a three-dimensional image of an LBD according to the present invention in an agonistic conformation, and

(b) the computer-aided modelling of chemical compounds with structures which are capable of undergoing specific interactions with an LBD in an agonistic conformation.

A method of finding active compounds for crop protection, in particular chemical compounds which, owing to binding to an LBD according to the present invention, bring about the activation or inhibition of USP, with the following steps:

(a) carrying out one of the abovementioned methods for finding USP ligands,

(b) synthesizing the compound(s) identified as ligands, and

(c) detecting the bioactivity of the compound synthesized in step (b) by transactivation assays, displacement assays or bioassays.

A method of finding active compounds for crop protection, in particular chemical compounds which, owing to binding to an LBD according to the present invention in an agonistic conformation, bring about the activation or inhibition of USP, with the following steps:

(a) carrying out one of the abovementioned methods for finding USP-LBD ligands in an agonistic conformation,

(b) synthesizing the compound(s) identified as ligands, and

(c) detecting the bioactivity of the compound synthesized in step (b) by transactivation assays, displacement assays or bioassays.

A method of finding effectors for systems for the inducible expression of target genes by means of USP, with the following steps:

(a) carrying out one of the abovementioned methods for finding USP ligands,

(b) synthesizing the compound(s) identified as ligands,

(c) applying a compound synthesized in step (b) to host cells or host organisms which contain a USP-based expression system, and

(d) detecting an induction or inhibition of the expression system.

The use of an LBD according to the present invention or of a computer-readable data storage medium according to the present invention for finding active compounds for crop protection or effectors for the controlled expression of target genes in host cells or intact host organisms.

The present invention is described in greater detail with reference to the examples which follow.

Examples

Example 1

Protein expression and purification

The Heliothis virescens USP-LBD (AS Val-205 to Met 466) was cloned in a pET-15b expression vector as N-terminal fusion protein with a His-tag and overexpressed in the E. coli strain BL21(DE3). The cells were cultured in 2x LB medium at 37°C and induced for 2 hours with 0.8 mM isopropyl-β-D-thiogalactopyranoside at 24°C. The protein extract was purified over a cobalt chelate column with subsequent gel filtration over a Superdex 200 16/60 column. The His-tag was then removed by digestion with thrombin and the protein was removed by gel filtration. A homogeneous monomeric protein species was present in the solution and was confirmed by means of SDS and native polyacrylamide gel electrophoresis and by denaturing and native electrospray ionization mass spectrometry.

Crystallization

Crystallization was effected by gas diffusion on hanging drops. The protein concentration employed was 3-9 mg/ml. Crystals 200 x 200 x 400 mm^3 in size formed within 10 days from a solution containing 10% of polyethylene glycol (PEG) 4000, 50 mM Tris (pH 7.5), 100 mM NaCl and 5 mM dithiothreitol and which was equilibrated in the reservoir against a solution of 20% polyethylene glycol (PEG) 4000 and 100 mM Tris (pH 7.5). The crystals belong to the tetragonal $P4_322$ spatial group with one monomer per asymmetric unit. The parameters of the standard cell are a=58.21 Å, b=58.21 Å, c=144.69 Å and $\alpha=\beta=\gamma=90°$. The solvent content is 32%, and the B-factor estimated in the Wilson Plot is 27 $Å^2$.

Data gathering, structure determination and refining

Crystals were immersed briefly in a 10% glycerol solution and shock-frozen in liquid nitrogen. The native data set was produced with a single crystal at measuring station ID14-EH2 at the ESRF (Grenoble, France). The data were processed with the aid of HKL programs (18). The crystal structure was solved by the molecular replacement method (19) by means of a partial hRXRα structure (20) as search model. A poor solution was achieved with a correlation of 24.8% and R_{free}=54.5% after refining as a rigid body. The phasing power of the model was low and required a number of manual generateing cycles with O (21). The wARP method (22) was used to verify the correctness of the partially-built structures. Refining was performed with CNS (23) using a maximum likelihood target function and solvent correction. Cycles of manual modelling and least-square minimization with subsequent simulated annealing and individual anisotropic B-factor refining gave rise to the final model. Solvent molecules were contoured in an $F_o - F_c$ map at a surface of 3σ. The final model, refined to a resolution of 1.65 Å, comprises 246 amino acid residues, 259 water molecules and one ligand molecule. A large portion of the connecting loop between Helix H5 and the beginning of the β-pleated sheet (amino acid residues 306-315) and the C-terminal extension of H12 (amino acid residues 459-466) could not be shown, owing to the poor electron density in these regions. The quality of the final model was checked with Procheck (24).

Characterization of the USP-LBD crystals by electrospray time-of-flight mass spectrometry (ESI TOF-MS) under natural conditions shows a heterogeneous mass distribution around 740 ± 50 Da in addition to the peak of the pure protein (30.2 kDa). This suggested that a ligand is present which is bound in LBD. The presence of a ligand was confirmed by the electron density. Various complementary techniques were used to characterize the ligand. The ligand, which is located in the binding pocket of the USP-LBD, was characterized as a phospholipid molecule. A phosphatidylglycerol or a phosphatidylethanolamine or a phosphatidylcholine would match the crystallographic data and are consistent with the results from mass

spectroscopy and chemical analysis. These amphiphilic molecules have a head group consisting of a phosphorylglycerol or a phosphorylethanolamine group and a tail of two different fatty acids which are bonded to the glycerol-3-phosphate by ester bonds. A detailed description of the ligand and its interactions with the USP-LBD residues are given in the following text.

Example 2

Architecture of the Heliothis virescens USP-LBD

In general, the architecture of the USP-LBD exhibits canonic NR folding with 11 α-helices (H1, H3-H12) and two short β-strands (s1-s2). This structure was compared with two other crystal structures which have essential properties of NRs and which are closely related to the Heliothis virescens USP: the binding pocket of agonist-bound RXRα (hRXRα/9-cis RA) and antagonist-bound mice RXRα (msRXRα/oleic acid). Superposing the USP-LBD with the structure of the holo-RXRα -LBD was carried out with the aid of a least-square fit [LSQ]. In total, the secondary structural elements of the USP-LBD are capable of reasonably good superposition by those of the holo-RXRα-LBD. The root mean square deviation (r.m.s.d.) is 1.22 Å for 183 out of 246 superposed Cα atoms. Seven helices are accessible to reasonably good superposition (r.m.s.d. 1.13, 0.88, 0.57, 1.18, 0.67, 0.69, 0.75 Å for H4, H5, H7-H11). The C-terminus of H1 is curved by approximately 2 Å relative to helix H3, and its r.m.s.d. is 1.63 Å. H3, H6 and the β-pleated sheet show larger deviations. The structure of the USP-LBD demonstrates that the activation helix H12 assumes a conformation which is similar to that of the antagonist-RXRα. The antagonistic AF-2 conformation of the USP-LBD is discussed further below.

The connecting loop L1-3 of most NRs usually behaves as a highly flexible region. In the case of hRXRα, the crystal structures of both the apo and the holo conformations show substantial differences in the regions which connect helices H1 and H3. In the holo-LDB structure, L1-3 consists of an extended loop which extends

beyone the β-pleated sheet and a Ω-loop. The apo form contains an additional helix in this region which unfolds in the holo-form. During the transition from the apo-form to the holo-form, L1-3 undergoes substantial movement. In particular, the Ω-loop becomes oriented towards the opposite side of the protein centre. As has been proposed on the basis of the comparison of the two structures, L1-3 might act as a molecular spring which accompanies the conformational changes which are linked to ligand binding. For the ligand-bound RARγ-LBD, the conformation of L1-3 resembles that of the holo-RXRα. Interestingly, L1-3 for ER-LBDs follows a path other than in the case of holo-RXRα. It runs between helix H3 and the β-pleated sheet, packed tightly to the protein centre.

In the case of the USP-LBD, L1-3 assumes none of the conformations which are otherwise found in the other NRs. Its course (Val-220 to Pro-239) was derived unambiguously from the electron density maps. Only few residues at the beginning of the loop, namely Asp-222, Pro-223 and Ser-224, were treated as alanins owing to the poor electron density of the side chains. The temperature factors of these residues are therefore higher (60-64 $Å^2$) than those of the other amino acids of L1-3 (on average 36 $Å^2$ over L1-3). The first residues of L1-3 form a path which crosses helix H3 in the region Gln-256 to Val-262. The next residues (Glu-226 to Pro-234) form an extended loop which runs along H3, and, finally, the last five residues of L1-3 (Asp-235 to Pro-239) form a loop which has substantial similarity with the Ω-loop observed in the LBDs of RXRα and RARγ. L1-3 assumes quite a tight conformation which makes it possible to establish direct contacts with the residues of helices H3, H11 and H12 and to stabilize their actual positions. This is important in as far as these helices are those structural elements which are subject to the greatest conformational changes owing to ligand binding.

The particular conformation of L1-3 is not based on crystal packing effects. In the region of the loop L1-3 of RXRα-LBD, the USP-LBD interacts with its symmetry-equivalent molecule via the β-pleated sheets. It is extremely likely that this interaction takes place since L1-3 does not already occupy this region when the protein is

in solution. If, owing to packing effects, L1-3 would be forced to swing and to move away from a conformation which is similar to the actual conformation of RXRα, several elements of the secondary structure would have to move drastically from this hypothetical conformation to their final position. It is therefore highly unlikely that this drastic reorganization of all of the LBD takes place, in particular because L1-3 lies in a region of the LBD in which L1-3 establishes very specific interactions with adjacent elements of the secondary structure.

Directly linked to loop L1-3, helix H3 differs from its counterparts in RXRα both regard to length and with regard to the position of the N- and C-terminal portion . In Heliothis virescens USP, H3 starts at Pro-240 and is therefore one turn longer than H3 in the ligand-bound RXRα (start at RXRα-Pro-264). The residues of H3 in the middle portion of the helix assume almost identical positions compared with the positions of the corresponding residues in the apo- and holo-RXRα-LBDs. However, both N- and C-terminal regions are curved towards the exterior of the protein centre. The N-terminal region of H3 (Pro-240 to Cys-250) is shifted substantially towards H11. It is tilted by approximately 24° in comparison with the same region in the holo-RXRα (approx. 7.2 Å between USP-Pro-245 and holo-RXRα-Pro-264). This position lies between those of the N-terminal regions in the apo-RXRα and the holo-RXRα-LBD structure. The outwardly curved C terminus of H3 (by approx. 10°) has effects on the arrangement of the adjacent loops L3-4 and L8-9. Loop L3-4, which is part of the signature region of NRs, is shifted laterally by approximately 1.8 Å and curved towards L8-9, while loop L8-9 itself is shifted outwardly by approximately 1.5 Å.

Example 3

The ligand-binding pocket

The ligand-binding pocket of Heliothis virescens USP is formed by residues of loop L1-3, helices H3, H5, H6 and H7, the β-pleated sheet and loop L11-12. As described

above, the N-terminal portion of helix H3 is markedly shifted outwardly compared with its opposite number in RXRα. Two other secondary structures which contribute to the binding pocket also differ from those in RXRα: 1) Helix 6 has moved inwardly by approximately 1.9 Å, and 2) the curvature of the β-pleated sheet points towards H1. The shift of the three structural elements which this entails lead to a widening of the ligand-binding pocket compared with that of the RXRα-LBD. The edge of the binding pocket is formed by the Ω-loop of L1-3, the N terminus of H3 and H6, while in the case of RXRα the opening of the pocket is formed by loop L11-12 and H6. At its opening, the binding pocket is approximately 13.5 Å wide (distance between Lys-241 in H3 and Gln-338 in H6). This opening is much wider than in the case of RXRα (7,1 Å from Pro-264 in H3 to Ala-340 in H6). The topology of the ligand-binding pocket is relatively unusual with a gap between H3 and H6. In RXRα and other NRs, this region forms fixed contacts with the connecting loop L1-3. The volume of the cavity of the USP-LBD achieves that of the hRXRα-LBD by a factor of 2.5 (1256 $Å^3$ in the case of USP compared with 489 $Å^3$ in the case of hRXRα).

Example 4

The putative ligand of USP in the crystal structure

Unexpectedly, the ligand-binding pocket of Heliothis virescens USP contains a molecule which was copurified and cocrystallized together with the USP-LBD. The fit of the electron density agrees well with the characterization of the molecules by mass spectroscopy and analytical chemistry. Similarly, recent crystallographic studies of the heterodimeric RARα/RXRα-LBD show an E.coli-endogenous oleic acid (C18) or a similar compound (stearic (C18) or palmitic (C16) acid) in the RXRα subunit. Even though this molecule is not the natural ligand of vertebrate NR, it induces and stabilizes an antagonistic AF-2 conformation which in all probability is very similar to the actual antagonist-bound RXRα.

In the present case, the best fit of the electron density was assumed with the assumption of a phospholipid whose first tail consists of a fatty acid with a length of 18 carbon atoms at C1 and a second chain at C2 which is 16 carbon atoms in length. The longer fatty acid of the two has a relatively twisted shape with two largish peaks, while the other fatty acid assumes a more normal form within the pocket. The tail of the phospholipid is hidden within the ligand-binding pocket. The glycerol moiety and the two fatty acids form van-der-Waals contacts with the residues in L1-3 (Leu-230, Val-238), H3 (Phe-242, Leu-249), H5 (Leu-291), L6-7 (Ala-339), H7 (Phe-345), H11 (Ser-431, His-434, Phe-438) and L11-12 (Leu-440). The head group of the phospholipid is positioned at the front at the opening of the pocket between H3 and H6. A strong hydrogen bond with Gln-338 (H6) is formed by the carbonyl group of the phosphorylglycerol in the case of phosphatidylglycerol and by the amino group of the ethanolamine in the case of phosphatidylethanolamine. In addition, an oxygen of the phosphate group is bound to a residue L1-3 (Cγ of Pro-239) by a hydrogen bridge.

It is assumed that the phospholipid found herein constitutes no natural USP ligands. However, it is shown unambiguously that USP ligands exist.

The residues which interact with the ligands are highly conserved within lepidopteran USPs, with the exception of Ser-431, which is replaced by a cysteine in msUSP. In contrast, among the 16 residues of the RXRα-LBD which interact with 9-cis RA, only 3 of the corresponding USP residues interact with the phospholipid (Leu-249, Ser-431 and His-434). The reason for this behaviour is mainly the different position of the ligands in the corresponding pockets. The 9-*cis* RA is very deep within the pocket, where its carboxylate group forms a salt bridge to Arg-316 of helix H5 of the hRXRα. In contrast, the phospholipid does not penetrate far into the inside of the pocket. For example the tail of the longer fatty acid lies approximately at atom C9 of 9-*cis* RA in hRXRα-LBD, while the tail of the other fatty acid extends almost to the β-ionone ring of 9-*cis* RA. As a consequence, Arg-297 does not participate in the anchorage of the ligand, as is observed in the case of the agonistic RXRα–, RARγ–

and other NR-LBDs. Nevertheless, it assumes almost the same position as Arg-316 of the holo-RXRα and not the position of the apo-RXRα conformation, which is exposed to the solvent. Instead of interacting with the ligand, Arg-297 forms hydrogen bonds with the backbone carbonyl group of Leu-325 (β-pleated sheet) and participates in a hydrogen bond network with Leu-290 (H5) and the side chain of Gln-256 (H3), with participation of water. In particular, two water molecules which are positioned spatially approximately at the two oxygen atoms of the carboxylate group of 9-*cis* RA participate in these interactions.

Example 5

The antagonistic conformation of the USP-LBD

The AF-2 domain in the structure of the USP-LBD exhibits an antagonistic conformation generated by the ligands in the ligand-binding pocket. H12 assumes the same conformation which has been found in the case of other antagonist-bound nuclear receptors such as RXRα /oleic acid, RARα/BMS614 and ER. In all these cases, it is observed that the groove in which H12 is positioned corresponds to the binding site for the helical nuclear receptor box of nuclear receptor coactivators. This helical nuclear receptor box is distinguished by the consensus sequence LXXLL, as has been shown for the ligand-binding domain of PPARγ, TRβ and ERα. In the case of the Heliothis virescens USP, Ile-450, Ala-453 and Leu-454 of H12 are approximately in the same position as the first, second and third leucin residue of the LXXLL binding motif (IXXAL instead of LXXLL). As in other antagonistic conformations of nuclear receptors, H12 is packed into a groove of residues of H3 and H4 and of L3-4 (Val-261, Arg-265, Met-275, Glu-276, Ile-279, Ile-282, Lys-283). However, in the case of the USP-LBD, L1-3 is also involved in the groove entopology and, with the residues Phe-227, Gln-228 and Phe-229, has van-der-Waals contacts with H12.

The length of H12 in the USP-LBD is identical to that of H12 in the antagonist-bound form of the RXRα-LBD. However, the structural principle which has been observed in another case of an antagonistic conformation of a nuclear receptor ligand-binding pocket is not found in its entirety in the case of the USP-LBD. Indeed, it has been found there that H11 coils up and thus permits H12 to bind to the binding groove of the nuclear receptor coactivator binding motif LXXLL. H11 is located in the extension of H10 and superposes very readily with H11 in the holo-RXRα-LBD structure, with the exception that the H11 of the USP-LBD is shorter by two residues. This is followed by a region 6 residues in length which connects H11 and H12 (His-439 to Thr-444). These amino acids of loop L11-12 span, in an extended conformation, a strand 12 Å in length. The C terminus of H11 contains three phenylalanins which are also found in RXRα. In apo-RXRα, the first two phenylalanins point towards the hydrophobic ligand-binding pocket while the third phenylalanin faces the solvent. In the agonist-bound form, the phenylalanins swap roles. In the USP-LBD, the situation is similar to the agonist-bound form of the RXRα-LBD: Phe-436 and Phe-437 face the solvent, while Phe-438 contributes to the ligand-binding pocket. In comparison with its counterpart in RXRα, the side chain of Phe-438 is rotated slightly and touches the ligand at the level of its shorter fatty acid. In the antagonist-bound form of RXRα, the first residue of the phenylalanin triplet corresponds to the end of H11. This residue is in approximately the position of the C-α atom of Phe-437. In the ligand-binding pocket, the two other phenylalanin residues, which are already part of L11-12, are orientated inwardly towards the inside of the protein. In a superposition of the Heliothis virescens USP and the antagonist-bound RXRα-LBD, these two residues collide with the phospholipid ligands.

Example 6

The connecting region L1-3 interacts with H3 and L11-12 and prevents an agonistic conformation

The binding of the phospholipid in the ligand-binding pocket of the USP-LBD probably generates important structural rearrangements in the USP-LBD. The comparison with apo- and holo-RXRα-LBD structures allows the assumption that in the USP-LBD, too, the molecular mechanisms which bring about the ligand-bound LBD conformation comprise the displacement of H3 and H11. However, in contrast to all other nuclear receptor LBDs known to date, the structural element L1-3 plays an essential role in the Heliothis virescens USP.

Loop L1-3 interacts with H3, H11, L11-12 and H12. These structural elements are most effective by the ligand binding. L1-3 stabilizes the N-terminus of H3 via a hydrogen bridge network with Arg-243 and Asn-254 of H3. The guanidinium moiety of the Arg-243 is anchored to the backbone carbonyls of Gly-233, Ser-236 and Val-238 by strong hydrogen bridges (distances 2.61, 2.97 and 2.78 Å, respectively) and shows a van-der-Waals contact with the side chain of Val-232. In addition, the backbone amide group of the Arg-243 is bound to the carbonyl group of Pro-239 (3.20 Å) by a hydrogen bond. The side chain of Asn-254 forms hydrogen bonds with the carbonyl group of Leu-230 (2.83 Å), to the amide group of Phe-229 (3.10 Å) and, via a water molecule, to the side chain of Gln-228. Moreover, it is in van-der-Waals contact with the carbonyl group of Phe-227. The backbone carbonyl group of Asn-254 forms a strong hydrogen bridge to the side chain of Glu-226 (2.74 Å).

L1-3 (Gln-228 to Arg-231, Asp-235 and Ser-236) is also in contact with N-terminal region of H11 and with L11-12. The backbone carbonyl group of Gln-228 forms a hydrogen bond with Ala-442 (3.20 Å), and the backbone carbonyl group of Phe-229 forms a strong hydrogen bridge with the amide group of Ala-442 (2.88 Å). In addition, Arg-231 stabilizes the loop L11-12 by means of strong interactions: the

backbone amide group forms a strong hydrogen bond with the carbonyl group of Leu-440 (2.90 Å), while the side chain forms a strong hydrogen bond with the carbonyl group of His-439 (3.00 Å) and shows van-der-Waals contacts with Val-441 and Ala-442. Other interactions concern the backbone carbonyl of Asp-235 with the side chain of His-439 and a water-mediated interaction with Val-441. The hydroxyl group of Ser-236 forms a van-der-Waals contact with the side chain of Leu-440.

It is important to state that a high degree of sequence conservation exists in all residues which participate in the interaction of L1-3 with H3 and with L11-12. The main interaction partners of H3, Arg-243 and Asn-254, are conserved strictly in all lepidopteran USPs. Likewise all interaction partners in L1-3 (Glu-226, Phe-227, Gln-228, Phe-229, Leu-230, Val-232, Gly-233, Ser-236, Val-238, Pro-239) are conserved strictly in all lepidopteran USPs, with the exception of Phe-227 and Phe-229, which are replaced by leucine and isoleucine in the Bombyx mori USP. In the case of the interactions of L1-3 with L11-12, too, the residues involved (L1-3: Gln-228 to Arg-231, Asp-235 and Ser-236; L11-12: His-439 to Ala-442) are conserved strictly in all lepidopteran USPs, with the exception of Phe-229 and Asp-235. This strongly suggests that interaction patterns of L1-3 with H3 and of L1-3 with L11-12 are similar in all lepidopteran USPs.

In the superposition of Heliothis virescens USP with the holo-RXRα-LBDs, it can be observed that some residues from L1-3 are approximately in the same position in the Heliothis virescens USP (Asn-237, Ser-236 and Phe-229), such as residues from L11-12 of holo-RXRα (Asp-444, Thr-445 and Phe-450). This comparison permits the informative conclusion that L1-3 in its actual conformation excludes the existence of an agonistic conformation since this would be hindered at loop L11-12. In any case, this is no crystallization artefact and reflects the particular role of this structural element in the lepidopteran USPs.

The sterical hindering of the agonistic position of H12 here is a constitutive component of the receptor structure and not the consequence of the bulky shape of

the ligand, as is the case in other nuclear receptor LBDs which are occupied by fully antagonistic ligands.

It can be predicted that ligand binding of agonists generates a change in the conformation of the USP-LBD, which makes L1-3, H12 and the other LBD residues which have been described jump into an antagonistic position.

In any case, this is not a crystallization artefact and constitutes the particular role of this structural element in the lepidopteran USPs.

Example 7

Agonistic conformation of the Heliothis virescens USP-LBD by homology modelling, based on the RXRα/9-cis-RA complex

In order to generate a 3D model of the Heliothis virescens USP-LBD, the lacking residues of the loop between helices H1 and H3 (L1-3) were complemented from the hRXRα crystal structure in such a way that a continuous backbone is formed. The resulting structure is the experimental hRXRα reference model.

Two hRXRα monomers were observed in the hRXRα standard cell, and the L1-3 region was poorly resolved in each of these monomers. Superposition of the two structures, which had been refined independently of one another, led to a suggestion as to where this loop should be modelled. A complete 3D model of hRXRα based on crystal structure and in which the residues in L1-3 are completed was built. The hydrogen atoms were completed with the aid of the Hgenerate option of the Charmm program.

The L1-3 region was relaxed by Powell minimization of the Charmm program (1000 optimization steps, dielectric constant : 4, gradient tolerance : 10^{-6}, step width 0.02, cutoff for non-binding interactions: 15 Å).

This optimized structure was used as template for the homology model of the Heliothis virescens USP-LBD.

The amino acid sequences of the Heliothis virescens USP-LBD and of hRXRα were assigned in accordance with Table 2.

With the aid of the software package Modeller and its standard settings, a 3D model was built with the aid of the assignment. The USP-LBD sequence shows a few insertions in loop 1-3 and in the loop before the first ß-pleated sheet. In order to establish meaningful conformations for these two regions, the option lego-loop of the software package O was used. The USP model structure was subsequently subjected to Powell minimization (2000 optimization steps, dielectric constant: 4, gradient tolerance: 10^{-6}, step width 0.02, cutoff for non-binding interactions: 15 Å). The quality of the structure thus obtained is analyzed with the program PROCHECK. Accordingly, 97% of the residues are in permitted regions and less than 2% of the residues are in prohibited regions. The latter are in the above-described modified regions.

Example 8

Comparison between the agonistic USP-LBD structure obtained from the hRXRα/9-cis RA complex and the USP-LBD crystal structure

The largest differences between these two structures are in the position of the activation helix (H12) and the path of the loop between the helices H1 and H3. The activation helix H12 is located in the experimental structure in the antagonistic position, while in the model structure it assumes an agonistic conformation which closes the ligand-binding niche. In the experimental structure, the loop L1-3 lies above the helix H3 and stabilizes the antagonistic position of H12 by hydrophobic contact. In contrast, this loop lies at a considerable distance from the central AFS-AD

helix in the agonistic homology model. Loop L1-3 is separated from helix H3 by the ß-pleated sheet.

Moreover, the size of the ligand-binding niche differs substantially between the two structures. The presence of the large fatty acid residue in the USP-LBD crystal structure causes a great cavity by shifting helices H3, H6 and H11. In the USP agonistic conformation, these helices are packed densely and produce a smaller ligand-binding niche.

The regions of the C-terminal ends of H3, H4, H5, H8 and H9 are rigid and capable of very good superposition in the two structures. In contrast, loop L1-3 and the C-termini of H3, H6 and H11 in the two structures are displaced relative to each other. These segments form the most mobile region of the ligand-binding domain of nuclear receptors. This movement is probably specific for each receptor and the ligand-generated displacement.

Information on the sequence listing

SEQ ID NO: 1 shows the amino acid sequence of the Heliothis virescens USP-LBD.

SEQ ID NO: 2 shows the amino acid sequence of the Heliothis virescens USP.

Information on the Tables

Table 1 shows the structure coordinates of the LBD of the Heliothis virescens USP.

Table 2 shows the amino acid sequence assignment for hRXRα and USP of Heliothis virescens and of further nuclear receptor LBDs for generateing a homology model of the agonistic USP conformation.

Table 1

REMARK coordinates from restrained individual B-factor refinement
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REMARK final r= 0.2112 free_r= 0.2459
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REMARK B rmsd for bonded sidechain atoms= 2.272 target= 2.0
REMARK B rmsd for angle mainchain atoms= 2.299 target= 2.0
REMARK B rmsd for angle sidechain atoms= 3.310 target= 2.5
REMARK rweight= 0.1000 (with wa= 1.12122)
REMARK target= mlf steps= 30
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REMARK parameter file 1 : CNS_TOPPAR:protein_rep.param
REMARK parameter file 2 : CNS_TOPPAR:water_rep.param
REMARK parameter file 3 : eph.par
REMARK molecular structure file: alternate.mtf
REMARK input coordinates: anneal_2.pdb
REMARK reflection file= /home/billas/USP/SCALE0400/merge1A65/usp_20a1a65.10.cv
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 1.65
REMARK initial B-factor correction applied to fobs :
REMARK B11= -1.985 B22= -1.985 B33= 3.970
REMARK B12= 0.000 B13= 0.000 B23= 0.000
REMARK B-factor correction applied to coordinate array B: -0.193
REMARK bulk solvent: density level= 0.33501 e/A^3, B-factor= 48.7849 A^2
REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected

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REMARK theoretical total number of refl. in resol. range:    30842 ( 100.0 % )
REMARK number of unobserved reflections (no entry or |F|=0):  1417 (  4.6 % )
REMARK number of reflections rejected:                           0 (  0.0 % )
REMARK total number of reflections used:                     29425 ( 95.4 % )
REMARK number of reflections in working set:                 26453 ( 85.8 % )
REMARK number of reflections in test set:                     2972 (  9.6 % )
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ATOM  170 CB  GLU  226    21.858 29.513 67.196 1.00 49.61
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ATOM 171 CG GLU 226 20.778 28.525 67.641 1.00 49.78
ATOM 172 CD GLU 226 19.333 28.959 67.359 1.00 51.91
ATOM 173 OE1 GLU 226 18.452 28.312 67.956 1.00 50.08
ATOM 174 OE2 GLU 226 19.039 29.909 66.543 1.00 51.77
ATOM 175 C GLU 226 21.015 31.344 68.670 1.00 46.28
ATOM 176 O GLU 226 21.839 31.794 69.476 1.00 47.17
ATOM 177 N PHE 227 19.733 31.155 68.942 1.00 41.52
ATOM 178 CA PHE 227 19.138 31.503 70.206 1.00 38.73
ATOM 179 CB PHE 227 17.723 32.022 69.963 1.00 40.03
ATOM 180 CG PHE 227 17.640 33.061 68.876 1.00 40.91
ATOM 181 CD1 PHE 227 17.775 32.703 67.542 1.00 40.72
ATOM 182 CD2 PHE 227 17.464 34.402 69.192 1.00 42.62
ATOM 183 CE1 PHE 227 17.739 33.661 66.535 1.00 42.04
ATOM 184 CE2 PHE 227 17.426 35.374 68.188 1.00 42.27
ATOM 185 CZ PHE 227 17.564 34.996 66.857 1.00 42.02
ATOM 186 C PHE 227 19.119 30.339 71.174 1.00 34.83
ATOM 187 O PHE 227 19.218 29.178 70.778 1.00 34.52
ATOM 188 N GLN 228 18.982 30.687 72.445 1.00 33.69
ATOM 189 CA GLN 228 18.979 29.735 73.540 1.00 32.01
ATOM 190 CB GLN 228 19.290 30.468 74.847 1.00 34.80
ATOM 191 CG GLN 228 20.680 31.080 74.935 1.00 39.39
ATOM 192 CD GLN 228 21.768 30.029 74.916 1.00 40.63
ATOM 193 OE1 GLN 228 22.117 29.504 73.860 1.00 44.27
ATOM 194 NE2 GLN 228 22.301 29.706 76.093 1.00 42.65
ATOM 195 C GLN 228 17.678 28.974 73.736 1.00 28.92
ATOM 196 O GLN 228 17.035 29.174 74.750 1.00 28.29
ATOM 197 N PHE 229 17.283 28.120 72.794 1.00 28.04
ATOM 198 CA PHE 229 16.056 27.340 72.996 1.00 25.30
ATOM 199 CB PHE 229 15.767 26.411 71.821 1.00 27.02
ATOM 200 CG PHE 229 15.066 27.055 70.680 1.00 28.71
ATOM 201 CD1 PHE 229 15.599 28.170 70.052 1.00 28.96
ATOM 202 CD2 PHE 229 13.903 26.480 70.173 1.00 30.61
ATOM 203 CE1 PHE 229 14.991 28.708 68.918 1.00 29.32
ATOM 204 CE2 PHE 229 13.284 26.998 69.046 1.00 31.44
ATOM 205 CZ PHE 229 13.829 28.117 68.412 1.00 31.43
ATOM 206 C PHE 229 16.276 26.434 74.195 1.00 23.81

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ATOM  207  O   PHE  229     15.385  26.202  75.014  1.00 22.15
ATOM  208  N   LEU  230     17.487  25.899  74.263  1.00 20.44
ATOM  209  CA  LEU  230     17.848  24.964  75.302  1.00 21.42
ATOM  210  CB  LEU  230     18.255  23.631  74.650  1.00 20.34
ATOM  211  CG  LEU  230     17.191  22.855  73.834  1.00 22.70
ATOM  212  CD1 LEU  230     17.860  21.762  73.013  1.00 23.14
ATOM  213  CD2 LEU  230     16.130  22.252  74.773  1.00 21.55
ATOM  214  C   LEU  230     19.017  25.540  76.094  1.00 20.71
ATOM  215  O   LEU  230     19.977  26.038  75.524  1.00 20.61
ATOM  216  N   ARG  231     18.931  25.467  77.411  1.00 20.48
ATOM  217  CA  ARG  231     20.018  25.997  78.211  1.00 20.62
ATOM  218  CB  ARG  231     20.023  27.525  78.176  1.00 20.50
ATOM  219  CG  ARG  231     18.907  28.184  79.017  1.00 24.52
ATOM  220  CD  ARG  231     17.560  28.025  78.342  1.00 27.62
ATOM  221  NE  ARG  231     16.465  28.674  79.060  1.00 28.14
ATOM  222  CZ  ARG  231     15.846  28.165  80.118  1.00 28.35
ATOM  223  NH1 ARG  231     16.208  26.986  80.598  1.00 27.27
ATOM  224  NH2 ARG  231     14.856  28.835  80.692  1.00 28.94
ATOM  225  C   ARG  231     19.957  25.585  79.663  1.00 20.62
ATOM  226  O   ARG  231     18.884  25.350  80.219  1.00 20.08
ATOM  227  N   VAL  232     21.138  25.549  80.265  1.00 20.70
ATOM  228  CA  VAL  232     21.276  25.244  81.684  1.00 23.23
ATOM  229  CB  VAL  232     22.596  24.499  81.961  1.00 24.57
ATOM  230  CG1 VAL  232     22.800  24.335  83.460  1.00 24.88
ATOM  231  CG2 VAL  232     22.565  23.135  81.289  1.00 23.34
ATOM  232  C   VAL  232     21.306  26.619  82.359  1.00 25.86
ATOM  233  O   VAL  232     22.284  27.349  82.225  1.00 29.87
ATOM  234  N   GLY  233     20.232  26.960  83.062  1.00 24.64
ATOM  235  CA  GLY  233     20.137  28.249  83.730  1.00 26.40
ATOM  236  C   GLY  233     20.170  28.129  85.240  1.00 27.72
ATOM  237  O   GLY  233     20.449  27.041  85.755  1.00 26.07
ATOM  238  N   PRO  234     19.863  29.206  85.980  1.00 28.00
ATOM  239  CD  PRO  234     19.340  30.507  85.515  1.00 30.45
ATOM  240  CA  PRO  234     19.886  29.158  87.447  1.00 28.48
ATOM  241  CB  PRO  234     19.772  30.627  87.833  1.00 30.42
ATOM  242  CG  PRO  234     18.804  31.123  86.802  1.00 32.04
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ATOM  243  C   PRO  234     18.752  28.323  88.037  1.00 27.91
ATOM  244  O   PRO  234     18.781  27.975  89.229  1.00 28.03
ATOM  245  N   ASP  235     17.757  27.996  87.210  1.00 26.13
ATOM  246  CA  ASP  235     16.636  27.186  87.680  1.00 23.93
ATOM  247  CB  ASP  235     15.333  27.686  87.064  1.00 28.77
ATOM  248  CG  ASP  235     15.405  27.820  85.544  1.00 31.24
ATOM  249  OD1 ASP  235     16.519  27.836  84.964  1.00 32.56
ATOM  250  OD2 ASP  235     14.327  27.922  84.919  1.00 34.70
ATOM  251  C   ASP  235     16.828  25.700  87.362  1.00 20.99
ATOM  252  O   ASP  235     16.019  24.881  87.751  1.00 19.94
ATOM  253  N   SER  236     17.914  25.369  86.666  0.50 20.63   AC1
ATOM  254  CA  SER  236     18.208  23.979  86.280  0.50 20.15   AC1
ATOM  255  CB  SER  236     19.196  23.969  85.111  0.50 19.44   AC1
ATOM  256  OG  SER  236     18.708  24.734  84.013  0.50 19.16   AC1
ATOM  257  C   SER  236     18.787  23.137  87.425  0.50 21.81   AC1
ATOM  258  O   SER  236     19.849  23.457  87.946  0.50 20.58   AC1
ATOM  259  N   ASN  237     18.125  22.037  87.782  1.00 21.94
ATOM  260  CA  ASN  237     18.621  21.202  88.886  1.00 25.34
ATOM  261  CB  ASN  237     17.498  20.331  89.450  1.00 30.84
ATOM  262  CG  ASN  237     17.020  19.301  88.472  1.00 34.04
ATOM  263  OD1 ASN  237     17.786  18.838  87.623  1.00 39.37
ATOM  264  ND2 ASN  237     15.748  18.913  88.588  1.00 39.05
ATOM  265  C   ASN  237     19.843  20.325  88.581  1.00 26.93
ATOM  266  O   ASN  237     20.180  19.405  89.339  1.00 32.05
ATOM  267  N   VAL  238     20.537  20.621  87.503  1.00 23.03
ATOM  268  CA  VAL  238     21.713  19.862  87.114  1.00 20.81
ATOM  269  CB  VAL  238     22.096  20.241  85.663  1.00 20.25
ATOM  270  CG1 VAL  238     23.336  19.495  85.207  1.00 19.20
ATOM  271  CG2 VAL  238     20.919  19.922  84.741  1.00 20.14
ATOM  272  C   VAL  238     22.844  20.185  88.106  1.00 20.62
ATOM  273  O   VAL  238     23.147  21.343  88.363  1.00 18.94
ATOM  274  N   PRO  239     23.428  19.153  88.719  1.00 20.32
ATOM  275  CD  PRO  239     23.144  17.726  88.541  1.00 20.40
ATOM  276  CA  PRO  239     24.515  19.328  89.688  1.00 21.49
ATOM  277  CB  PRO  239     24.911  17.892  90.023  1.00 22.13
ATOM  278  CG  PRO  239     23.696  17.174  89.847  1.00 20.51
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ATOM	279	C	PRO	239	25.663	20.039	89.023	1.00	24.59
ATOM	280	O	PRO	239	25.924	19.804	87.847	1.00	23.65
ATOM	281	N	PRO	240	26.388	20.879	89.777	1.00	24.92
ATOM	282	CD	PRO	240	26.142	21.311	91.167	1.00	26.02
ATOM	283	CA	PRO	240	27.524	21.603	89.202	1.00	26.88
ATOM	284	CB	PRO	240	28.222	22.161	90.438	1.00	26.73
ATOM	285	CG	PRO	240	27.039	22.543	91.299	1.00	29.18
ATOM	286	C	PRO	240	28.434	20.733	88.363	1.00	26.35
ATOM	287	O	PRO	240	28.847	21.125	87.259	1.00	27.72
ATOM	288	N	LYS	241	28.745	19.533	88.838	1.00	28.50
ATOM	289	CA	LYS	241	29.642	18.682	88.071	1.00	28.19
ATOM	290	CB	LYS	241	30.073	17.457	88.878	1.00	32.48
ATOM	291	CG	LYS	241	28.970	16.508	89.292	1.00	34.64
ATOM	292	CD	LYS	241	29.627	15.241	89.832	1.00	37.47
ATOM	293	CE	LYS	241	28.627	14.162	90.157	1.00	39.69
ATOM	294	NZ	LYS	241	29.359	12.932	90.578	1.00	42.50
ATOM	295	C	LYS	241	29.144	18.233	86.700	1.00	27.86
ATOM	296	O	LYS	241	29.935	17.790	85.868	1.00	27.57
ATOM	297	N	PHE	242	27.840	18.335	86.459	1.00	25.10
ATOM	298	CA	PHE	242	27.309	17.953	85.154	1.00	22.57
ATOM	299	CB	PHE	242	26.161	16.954	85.319	1.00	24.91
ATOM	300	CG	PHE	242	26.600	15.619	85.856	1.00	28.41
ATOM	301	CD1	PHE	242	27.411	14.790	85.102	1.00	30.20
ATOM	302	CD2	PHE	242	26.194	15.191	87.108	1.00	28.96
ATOM	303	CE1	PHE	242	27.813	13.544	85.583	1.00	31.58
ATOM	304	CE2	PHE	242	26.594	13.943	87.596	1.00	30.20
ATOM	305	CZ	PHE	242	27.400	13.127	86.832	1.00	32.03
ATOM	306	C	PHE	242	26.837	19.151	84.330	1.00	19.63
ATOM	307	O	PHE	242	26.386	18.991	83.190	1.00	20.79
ATOM	308	N	ARG	243	26.971	20.350	84.873	1.00	19.69
ATOM	309	CA	ARG	243	26.513	21.529	84.153	1.00	20.41
ATOM	310	CB	ARG	243	26.538	22.749	85.066	1.00	20.87
ATOM	311	CG	ARG	243	25.523	22.602	86.208	1.00	23.08
ATOM	312	CD	ARG	243	25.562	23.759	87.130	1.00	26.38
ATOM	313	NE	ARG	243	24.725	24.856	86.687	1.00	27.91
ATOM	314	CZ	ARG	243	23.394	24.873	86.728	1.00	28.35

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ATOM   315 NH1 ARG  243     22.697  23.825  87.192  1.00 26.91
ATOM   316 NH2 ARG  243     22.764  25.975  86.343  1.00 28.11
ATOM   317 C   ARG  243     27.238  21.813  82.846  1.00 20.13
ATOM   318 O   ARG  243     26.596  22.114  81.836  1.00 19.71
ATOM   319 N   ALA  244     28.564  21.734  82.838  1.00 20.90
ATOM   320 CA  ALA  244     29.273  21.974  81.577  1.00 22.06
ATOM   321 CB  ALA  244     30.773  21.896  81.796  1.00 21.20
ATOM   322 C   ALA  244     28.842  20.984  80.492  1.00 21.05
ATOM   323 O   ALA  244     28.527  21.365  79.366  1.00 21.57
ATOM   324 N   PRO  245     28.783  19.696  80.822  1.00 21.63
ATOM   325 CD  PRO  245     29.335  19.087  82.049  1.00 25.65
ATOM   326 CA  PRO  245     28.377  18.672  79.861  1.00 22.28
ATOM   327 CB  PRO  245     28.516  17.380  80.666  1.00 24.91
ATOM   328 CG  PRO  245     29.614  17.694  81.605  1.00 25.26
ATOM   329 C   PRO  245     26.943  18.859  79.329  1.00 19.49
ATOM   330 O   PRO  245     26.691  18.778  78.118  1.00 21.31
ATOM   331 N   VAL  246     26.013  19.123  80.230  1.00 20.18
ATOM   332 CA  VAL  246     24.624  19.294  79.805  1.00 18.44
ATOM   333 CB  VAL  246     23.693  19.269  81.028  1.00 18.35
ATOM   334 CG1 VAL  246     22.221  19.536  80.620  1.00 18.11
ATOM   335 CG2 VAL  246     23.766  17.845  81.678  1.00 17.69
ATOM   336 C   VAL  246     24.501  20.568  78.968  1.00 18.23
ATOM   337 O   VAL  246     23.773  20.603  77.977  1.00 18.23
ATOM   338 N   SER  247     25.234  21.609  79.351  0.50 20.08   AC1
ATOM   339 CA  SER  247     25.198  22.858  78.599  0.50 21.19   AC1
ATOM   340 CB  SER  247     26.058  23.910  79.289  0.50 21.37   AC1
ATOM   341 OG  SER  247     25.484  24.292  80.517  0.50 23.67   AC1
ATOM   342 C   SER  247     25.712  22.621  77.189  0.50 21.32   AC1
ATOM   343 O   SER  247     25.180  23.161  76.217  0.50 21.62   AC1
ATOM   344 N   SER  248     26.756  21.811  77.076  1.00 20.43
ATOM   345 CA  SER  248     27.322  21.502  75.766  1.00 21.62
ATOM   346 CB  SER  248     28.541  20.594  75.916  1.00 24.31
ATOM   347 OG  SER  248     29.660  21.350  76.354  1.00 24.89
ATOM   348 C   SER  248     26.271  20.800  74.903  1.00 22.36
ATOM   349 O   SER  248     26.158  21.061  73.697  1.00 22.32
ATOM   350 N   LEU  249     25.513  19.895  75.519  1.00 22.35
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ATOM	351	CA	LEU	249	24.462	19.185	74.791	1.00	22.28
ATOM	352	CB	LEU	249	23.904	18.046	75.668	1.00	22.23
ATOM	353	CG	LEU	249	24.970	16.972	75.954	1.00	25.52
ATOM	354	CD1	LEU	249	24.441	15.919	76.922	1.00	26.39
ATOM	355	CD2	LEU	249	25.398	16.341	74.643	1.00	27.01
ATOM	356	C	LEU	249	23.358	20.152	74.352	1.00	21.63
ATOM	357	O	LEU	249	22.822	20.039	73.231	1.00	19.99
ATOM	358	N	CYS	250	23.012	21.102	75.217	1.00	21.10
ATOM	359	CA	CYS	250	21.995	22.098	74.856	1.00	21.22
ATOM	360	CB	CYS	250	21.701	23.044	76.019	1.00	20.65
ATOM	361	SG	CYS	250	20.853	22.249	77.396	1.00	22.08
ATOM	362	C	CYS	250	22.471	22.932	73.684	1.00	22.49
ATOM	363	O	CYS	250	21.687	23.302	72.828	1.00	23.08
ATOM	364	N	GLN	251	23.765	23.239	73.656	1.00	22.61
ATOM	365	CA	GLN	251	24.313	24.064	72.577	1.00	24.50
ATOM	366	CB	GLN	251	25.738	24.482	72.925	1.00	26.13
ATOM	367	CG	GLN	251	25.827	25.428	74.123	1.00	31.89
ATOM	368	CD	GLN	251	27.270	25.602	74.609	1.00	36.32
ATOM	369	OE1	GLN	251	28.146	26.020	73.846	1.00	38.70
ATOM	370	NE2	GLN	251	27.520	25.275	75.883	1.00	36.33
ATOM	371	C	GLN	251	24.290	23.309	71.255	1.00	23.96
ATOM	372	O	GLN	251	24.080	23.899	70.200	1.00	25.04
ATOM	373	N	ILE	252	24.506	21.998	71.323	1.00	23.74
ATOM	374	CA	ILE	252	24.475	21.143	70.140	1.00	24.05
ATOM	375	CB	ILE	252	24.877	19.690	70.493	1.00	25.71
ATOM	376	CG2	ILE	252	24.385	18.727	69.419	1.00	25.12
ATOM	377	CG1	ILE	252	26.405	19.596	70.658	1.00	26.17
ATOM	378	CD1	ILE	252	26.874	18.335	71.359	1.00	27.45
ATOM	379	C	ILE	252	23.032	21.183	69.642	1.00	25.30
ATOM	380	O	ILE	252	22.760	21.312	68.448	1.00	25.88
ATOM	381	N	GLY	253	22.101	21.105	70.580	1.00	25.76
ATOM	382	CA	GLY	253	20.698	21.167	70.213	1.00	24.72
ATOM	383	C	GLY	253	20.327	22.497	69.573	1.00	24.98
ATOM	384	O	GLY	253	19.611	22.527	68.561	1.00	24.56
ATOM	385	N	ASN	254	20.779	23.600	70.165	1.00	23.66
ATOM	386	CA	ASN	254	20.483	24.929	69.642	1.00	24.18

ATOM	387	CB	ASN	254	21.063	25.999	70.566	1.00	23.04
ATOM	388	CG	ASN	254	20.336	26.061	71.884	1.00	24.90
ATOM	389	OD1	ASN	254	19.147	25.729	71.954	1.00	22.87
ATOM	390	ND2	ASN	254	21.020	26.511	72.934	1.00	25.39
ATOM	391	C	ASN	254	20.990	25.142	68.215	1.00	25.59
ATOM	392	O	ASN	254	20.349	25.832	67.418	1.00	25.49
ATOM	393	N	LYS	255	22.154	24.575	67.915	1.00	24.87
ATOM	394	CA	LYS	255	22.718	24.669	66.572	1.00	26.12
ATOM	395	CB	LYS	255	24.121	24.061	66.518	1.00	29.40
ATOM	396	CG	LYS	255	25.162	24.983	67.112	1.00	33.68
ATOM	397	CD	LYS	255	26.481	24.293	67.392	1.00	34.86
ATOM	398	CE	LYS	255	27.280	24.027	66.150	1.00	35.57
ATOM	399	NZ	LYS	255	28.719	23.853	66.527	1.00	33.75
ATOM	400	C	LYS	255	21.816	23.924	65.608	1.00	26.04
ATOM	401	O	LYS	255	21.539	24.415	64.507	1.00	25.57
ATOM	402	N	GLN	256	21.358	22.741	66.009	1.00	24.02
ATOM	403	CA	GLN	256	20.498	21.967	65.121	1.00	23.89
ATOM	404	CB	GLN	256	20.325	20.546	65.658	1.00	25.47
ATOM	405	CG	GLN	256	21.676	19.880	65.887	1.00	28.63
ATOM	406	CD	GLN	256	21.565	18.517	66.534	1.00	30.93
ATOM	407	OE1	GLN	256	20.710	18.301	67.387	1.00	32.63
ATOM	408	NE2	GLN	256	22.439	17.599	66.149	1.00	30.18
ATOM	409	C	GLN	256	19.156	22.658	64.915	1.00	24.45
ATOM	410	O	GLN	256	18.596	22.598	63.828	1.00	24.20
ATOM	411	N	ILE	257	18.662	23.338	65.942	1.00	23.21
ATOM	412	CA	ILE	257	17.390	24.059	65.816	1.00	22.41
ATOM	413	CB	ILE	257	16.895	24.535	67.180	1.00	20.26
ATOM	414	CG2	ILE	257	15.636	25.401	67.021	1.00	21.15
ATOM	415	CG1	ILE	257	16.607	23.298	68.039	1.00	22.12
ATOM	416	CD1	ILE	257	16.309	23.620	69.517	1.00	21.36
ATOM	417	C	ILE	257	17.558	25.253	64.877	1.00	23.91
ATOM	418	O	ILE	257	16.677	25.544	64.060	1.00	21.49
ATOM	419	N	ALA	258	18.684	25.949	64.994	1.00	23.86
ATOM	420	CA	ALA	258	18.939	27.081	64.103	1.00	25.37
ATOM	421	CB	ALA	258	20.313	27.705	64.416	1.00	26.26
ATOM	422	C	ALA	258	18.906	26.588	62.656	1.00	25.01

ATOM	423	O	ALA	258	18.306	27.238	61.783	1.00	25.91
ATOM	424	N	ALA	259	19.555	25.450	62.403	1.00	23.72
ATOM	425	CA	ALA	259	19.602	24.865	61.063	1.00	24.51
ATOM	426	CB	ALA	259	20.442	23.613	61.058	1.00	24.62
ATOM	427	C	ALA	259	18.187	24.525	60.623	1.00	24.36
ATOM	428	O	ALA	259	17.846	24.693	59.464	1.00	23.27
ATOM	429	N	LEU	260	17.374	24.015	61.544	1.00	23.02
ATOM	430	CA	LEU	260	15.986	23.685	61.188	1.00	24.75
ATOM	431	CB	LEU	260	15.237	23.070	62.366	1.00	26.22
ATOM	432	CG	LEU	260	15.550	21.633	62.742	1.00	31.27
ATOM	433	CD1	LEU	260	14.906	21.342	64.082	1.00	32.20
ATOM	434	CD2	LEU	260	15.054	20.679	61.658	1.00	33.32
ATOM	435	C	LEU	260	15.214	24.902	60.750	1.00	25.40
ATOM	436	O	LEU	260	14.391	24.821	59.834	1.00	23.40
ATOM	437	N	VAL	261	15.439	26.031	61.419	1.00	25.21
ATOM	438	CA	VAL	261	14.735	27.247	61.055	1.00	26.95
ATOM	439	CB	VAL	261	15.050	28.411	62.036	1.00	25.46
ATOM	440	CG1	VAL	261	14.386	29.700	61.544	1.00	27.40
ATOM	441	CG2	VAL	261	14.520	28.075	63.434	1.00	27.42
ATOM	442	C	VAL	261	15.104	27.671	59.640	1.00	26.53
ATOM	443	O	VAL	261	14.232	28.035	58.850	1.00	25.34
ATOM	444	N	VAL	262	16.396	27.611	59.320	1.00	27.29
ATOM	445	CA	VAL	262	16.874	27.995	57.993	1.00	28.11
ATOM	446	CB	VAL	262	18.430	27.910	57.905	1.00	30.08
ATOM	447	CG1	VAL	262	18.883	27.872	56.441	1.00	33.75
ATOM	448	CG2	VAL	262	19.051	29.104	58.606	1.00	32.97
ATOM	449	C	VAL	262	16.267	27.075	56.939	1.00	26.73
ATOM	450	O	VAL	262	15.909	27.511	55.840	1.00	26.28
ATOM	451	N	TRP	263	16.177	25.794	57.286	1.00	24.38
ATOM	452	CA	TRP	263	15.623	24.775	56.402	1.00	25.26
ATOM	453	CB	TRP	263	15.831	23.406	57.052	1.00	23.10
ATOM	454	CG	TRP	263	15.102	22.286	56.409	1.00	24.27
ATOM	455	CD2	TRP	263	13.881	21.697	56.873	1.00	24.86
ATOM	456	CE2	TRP	263	13.536	20.681	55.962	1.00	25.93
ATOM	457	CE3	TRP	263	13.051	21.936	57.974	1.00	24.53
ATOM	458	CD1	TRP	263	15.441	21.624	55.267	1.00	24.80

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ATOM   459 NE1 TRP  263     14.501  20.655  54.990  1.00 27.16
ATOM   460 CZ2 TRP  263     12.391  19.895  56.115  1.00 26.26
ATOM   461 CZ3 TRP  263     11.911  21.151  58.132  1.00 23.32
ATOM   462 CH2 TRP  263     11.598  20.144  57.204  1.00 23.73
ATOM   463 C   TRP  263     14.125  25.047  56.175  1.00 24.66
ATOM   464 O   TRP  263     13.645  25.081  55.037  1.00 25.81
ATOM   465 N   ALA  264     13.391  25.278  57.252  1.00 24.56
ATOM   466 CA  ALA  264     11.949  25.506  57.103  1.00 25.04
ATOM   467 CB  ALA  264     11.304  25.733  58.464  1.00 26.00
ATOM   468 C   ALA  264     11.675  26.701  56.205  1.00 27.22
ATOM   469 O   ALA  264     10.838  26.640  55.293  1.00 24.71
ATOM   470 N   ARG  265     12.372  27.794  56.489  1.00 28.16
ATOM   471 CA  ARG  265     12.227  29.024  55.724  1.00 32.11
ATOM   472 CB  ARG  265     13.250  30.066  56.218  1.00 33.47
ATOM   473 CG  ARG  265     13.155  31.408  55.520  1.00 36.25
ATOM   474 CD  ARG  265     14.169  32.397  56.078  1.00 39.06
ATOM   475 NE  ARG  265     15.545  31.972  55.823  1.00 42.06
ATOM   476 CZ  ARG  265     16.609  32.534  56.391  1.00 43.94
ATOM   477 NH1 ARG  265     16.447  33.541  57.244  1.00 44.49
ATOM   478 NH2 ARG  265     17.827  32.092  56.110  1.00 43.52
ATOM   479 C   ARG  265     12.424  28.767  54.225  1.00 32.76
ATOM   480 O   ARG  265     11.843  29.460  53.392  1.00 35.61
ATOM   481 N   ASP  266     13.227  27.771  53.872  1.00 33.71
ATOM   482 CA  ASP  266     13.465  27.492  52.466  1.00 34.17
ATOM   483 CB  ASP  266     14.931  27.106  52.236  1.00 37.32
ATOM   484 CG  ASP  266     15.879  28.293  52.374  1.00 40.62
ATOM   485 OD1 ASP  266     15.556  29.392  51.866  1.00 40.66
ATOM   486 OD2 ASP  266     16.959  28.128  52.985  1.00 43.94
ATOM   487 C   ASP  266     12.544  26.447  51.833  1.00 33.93
ATOM   488 O   ASP  266     12.664  26.156  50.646  1.00 32.38
ATOM   489 N   ILE  267     11.640  25.869  52.619  1.00 32.18
ATOM   490 CA  ILE  267     10.694  24.897  52.077  1.00 30.21
ATOM   491 CB  ILE  267      9.820  24.279  53.210  1.00 29.16
ATOM   492 CG2 ILE  267      8.586  23.588  52.620  1.00 31.21
ATOM   493 CG1 ILE  267     10.643  23.291  54.038  1.00 29.01
ATOM   494 CD1 ILE  267     11.069  22.051  53.278  1.00 28.89
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ATOM	495	C	ILE	267	9.800	25.670	51.093	1.00	30.06	
ATOM	496	O	ILE	267	9.256	26.715	51.421	1.00	29.41	
ATOM	497	N	PRO	268	9.653	25.164	49.862	1.00	31.41	
ATOM	498	CD	PRO	268	10.216	23.921	49.300	1.00	31.06	
ATOM	499	CA	PRO	268	8.813	25.857	48.879	1.00	31.62	
ATOM	500	CB	PRO	268	8.686	24.830	47.755	1.00	31.63	
ATOM	501	CG	PRO	268	10.012	24.126	47.811	1.00	34.16	
ATOM	502	C	PRO	268	7.459	26.286	49.444	1.00	31.83	
ATOM	503	O	PRO	268	6.762	25.483	50.051	1.00	31.61	
ATOM	504	N	HIS	269	7.128	27.566	49.267	1.00	31.08	
ATOM	505	CA	HIS	269	5.867	28.164	49.715	1.00	31.47	
ATOM	506	CB	HIS	269	4.677	27.277	49.300	1.00	33.82	
ATOM	507	CG	HIS	269	4.710	26.845	47.865	1.00	36.44	
ATOM	508	CD2	HIS	269	4.694	25.611	47.305	1.00	37.13	
ATOM	509	ND1	HIS	269	4.734	27.740	46.816	1.00	39.48	
ATOM	510	CE1	HIS	269	4.731	27.078	45.672	1.00	37.91	
ATOM	511	NE2	HIS	269	4.706	25.785	45.941	1.00	39.31	
ATOM	512	C	HIS	269	5.745	28.465	51.210	1.00	30.01	
ATOM	513	O	HIS	269	4.796	29.133	51.638	1.00	28.74	
ATOM	514	N	PHE	270	6.693	27.994	52.012	1.00	28.26	
ATOM	515	CA	PHE	270	6.607	28.222	53.454	1.00	27.87	
ATOM	516	CB	PHE	270	7.728	27.468	54.178	1.00	26.66	
ATOM	517	CG	PHE	270	7.661	27.563	55.684	1.00	24.18	
ATOM	518	CD1	PHE	270	6.867	26.683	56.415	1.00	24.15	
ATOM	519	CD2	PHE	270	8.385	28.536	56.372	1.00	26.34	
ATOM	520	CE1	PHE	270	6.792	26.775	57.822	1.00	22.45	
ATOM	521	CE2	PHE	270	8.316	28.637	57.778	1.00	24.45	
ATOM	522	CZ	PHE	270	7.516	27.754	58.494	1.00	23.03	
ATOM	523	C	PHE	270	6.650	29.707	53.811	1.00	28.65	
ATOM	524	O	PHE	270	5.866	30.175	54.634	1.00	29.19	
ATOM	525	N	SER	271	7.558	30.448	53.184	0.50	29.83	AC1
ATOM	526	CA	SER	271	7.676	31.876	53.463	0.50	31.34	AC1
ATOM	527	CB	SER	271	8.959	32.432	52.839	0.50	31.74	AC1
ATOM	528	OG	SER	271	10.104	31.869	53.460	0.50	31.64	AC1
ATOM	529	C	SER	271	6.458	32.663	52.974	0.50	32.85	AC1
ATOM	530	O	SER	271	6.301	33.839	53.296	0.50	33.99	AC1

ATOM	531	N	GLN	272	5.599	32.009	52.197	1.00	33.79
ATOM	532	CA	GLN	272	4.378	32.642	51.696	1.00	35.22
ATOM	533	CB	GLN	272	3.910	31.928	50.423	1.00	39.02
ATOM	534	CG	GLN	272	4.777	32.210	49.191	1.00	43.59
ATOM	535	CD	GLN	272	4.608	31.169	48.086	1.00	45.89
ATOM	536	OE1	GLN	272	3.488	30.794	47.727	1.00	47.68
ATOM	537	NE2	GLN	272	5.729	30.703	47.534	1.00	48.15
ATOM	538	C	GLN	272	3.255	32.633	52.742	1.00	35.20
ATOM	539	O	GLN	272	2.288	33.397	52.648	1.00	33.55
ATOM	540	N	LEU	273	3.383	31.756	53.736	1.00	33.18
ATOM	541	CA	LEU	273	2.402	31.651	54.811	1.00	31.26
ATOM	542	CB	LEU	273	2.695	30.398	55.653	1.00	30.14
ATOM	543	CG	LEU	273	2.671	29.015	54.988	1.00	29.04
ATOM	544	CD1	LEU	273	3.273	27.989	55.930	1.00	28.99
ATOM	545	CD2	LEU	273	1.231	28.638	54.645	1.00	29.21
ATOM	546	C	LEU	273	2.500	32.880	55.722	1.00	30.95
ATOM	547	O	LEU	273	3.556	33.513	55.793	1.00	30.58
ATOM	548	N	GLU	274	1.416	33.208	56.420	1.00	31.28
ATOM	549	CA	GLU	274	1.435	34.332	57.355	1.00	32.85
ATOM	550	CB	GLU	274	0.154	34.378	58.195	1.00	35.60
ATOM	551	CG	GLU	274	-1.039	35.022	57.511	1.00	40.50
ATOM	552	CD	GLU	274	-0.954	36.543	57.494	1.00	43.35
ATOM	553	OE1	GLU	274	-1.788	37.171	56.807	1.00	44.88
ATOM	554	OE2	GLU	274	-0.062	37.109	58.169	1.00	45.29
ATOM	555	C	GLU	274	2.615	34.079	58.287	1.00	32.91
ATOM	556	O	GLU	274	2.867	32.936	58.693	1.00	31.56
ATOM	557	N	MET	275	3.331	35.136	58.632	1.00	31.54
ATOM	558	CA	MET	275	4.483	35.010	59.507	1.00	31.78
ATOM	559	CB	MET	275	5.094	36.392	59.748	1.00	34.73
ATOM	560	CG	MET	275	6.288	36.403	60.673	1.00	37.61
ATOM	561	SD	MET	275	7.574	35.262	60.158	1.00	39.49
ATOM	562	CE	MET	275	7.940	35.869	58.496	1.00	39.54
ATOM	563	C	MET	275	4.149	34.351	60.838	1.00	31.91
ATOM	564	O	MET	275	4.885	33.474	61.305	1.00	31.90
ATOM	565	N	GLU	276	3.052	34.764	61.458	1.00	31.07
ATOM	566	CA	GLU	276	2.684	34.184	62.736	1.00	30.79

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ATOM   567  CB  GLU  276      1.499  34.938  63.341  1.00 35.06
ATOM   568  CG  GLU  276      1.866  36.382  63.755  1.00 37.66
ATOM   569  CD  GLU  276      3.043  36.434  64.731  1.00 40.34
ATOM   570  OE1 GLU  276      2.978  35.751  65.774  1.00 41.45
ATOM   571  OE2 GLU  276      4.034  37.157  64.464  1.00 42.59
ATOM   572  C   GLU  276      2.388  32.693  62.596  1.00 29.05
ATOM   573  O   GLU  276      2.529  31.946  63.559  1.00 28.93
ATOM   574  N   ASP  277      1.973  32.250  61.411  1.00 26.93
ATOM   575  CA  ASP  277      1.716  30.817  61.223  1.00 24.95
ATOM   576  CB  ASP  277      0.817  30.565  60.005  1.00 26.30
ATOM   577  CG  ASP  277     -0.656  30.768  60.320  1.00 26.04
ATOM   578  OD1 ASP  277     -0.984  31.102  61.476  1.00 29.19
ATOM   579  OD2 ASP  277     -1.492  30.596  59.410  1.00 26.42
ATOM   580  C   ASP  277      3.056  30.089  61.069  1.00 25.34
ATOM   581  O   ASP  277      3.226  28.967  61.579  1.00 25.43
ATOM   582  N   GLN  278      4.007  30.721  60.373  1.00 23.47
ATOM   583  CA  GLN  278      5.338  30.132  60.203  1.00 23.93
ATOM   584  CB  GLN  278      6.275  31.094  59.467  1.00 23.08
ATOM   585  CG  GLN  278      5.931  31.265  57.999  1.00 26.36
ATOM   586  CD  GLN  278      6.858  32.238  57.324  1.00 26.00
ATOM   587  OE1 GLN  278      8.075  32.122  57.439  1.00 26.10
ATOM   588  NE2 GLN  278      6.293  33.210  56.609  1.00 28.94
ATOM   589  C   GLN  278      5.917  29.850  61.588  1.00 22.78
ATOM   590  O   GLN  278      6.445  28.765  61.857  1.00 20.87
ATOM   591  N   ILE  279      5.821  30.849  62.461  1.00 23.32
ATOM   592  CA  ILE  279      6.322  30.719  63.825  1.00 22.80
ATOM   593  CB  ILE  279      6.125  32.046  64.591  1.00 24.62
ATOM   594  CG2 ILE  279      6.449  31.868  66.076  1.00 24.08
ATOM   595  CG1 ILE  279      6.997  33.125  63.943  1.00 27.52
ATOM   596  CD1 ILE  279      6.728  34.543  64.464  1.00 27.69
ATOM   597  C   ILE  279      5.638  29.560  64.573  1.00 22.81
ATOM   598  O   ILE  279      6.294  28.758  65.215  1.00 23.50
ATOM   599  N   LEU  280      4.318  29.463  64.498  1.00 20.16
ATOM   600  CA  LEU  280      3.653  28.382  65.186  1.00 18.30
ATOM   601  CB  LEU  280      2.125  28.553  65.113  1.00 19.64
ATOM   602  CG  LEU  280      1.589  29.739  65.931  1.00 22.60
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ATOM   603  CD1 LEU  280      0.093  29.931  65.623  1.00 24.59
ATOM   604  CD2 LEU  280      1.759  29.496  67.399  1.00 25.05
ATOM   605  C   LEU  280      4.045  27.028  64.653  1.00 17.14
ATOM   606  O   LEU  280      4.160  26.084  65.436  1.00 18.84
ATOM   607  N   LEU  281      4.225  26.905  63.335  1.00 17.52
ATOM   608  CA  LEU  281      4.586  25.591  62.773  1.00 19.05
ATOM   609  CB  LEU  281      4.550  25.618  61.241  1.00 19.60
ATOM   610  CG  LEU  281      3.167  25.782  60.595  1.00 21.40
ATOM   611  CD1 LEU  281      3.324  25.870  59.073  1.00 23.62
ATOM   612  CD2 LEU  281      2.266  24.621  60.975  1.00 21.20
ATOM   613  C   LEU  281      5.968  25.143  63.255  1.00 19.84
ATOM   614  O   LEU  281      6.164  23.977  63.620  1.00 19.38
ATOM   615  N   ILE  282      6.923  26.067  63.269  1.00 20.43
ATOM   616  CA  ILE  282      8.270  25.740  63.731  1.00 19.64
ATOM   617  CB  ILE  282      9.274  26.881  63.361  1.00 20.44
ATOM   618  CG2 ILE  282     10.619  26.706  64.102  1.00 20.04
ATOM   619  CG1 ILE  282      9.486  26.873  61.839  1.00 20.45
ATOM   620  CD1 ILE  282     10.278  28.076  61.323  1.00 22.03
ATOM   621  C   ILE  282      8.255  25.496  65.239  1.00 19.41
ATOM   622  O   ILE  282      8.894  24.574  65.717  1.00 19.21
ATOM   623  N   LYS  283      7.533  26.322  65.992  1.00 17.59
ATOM   624  CA  LYS  283      7.480  26.148  67.446  1.00 19.01
ATOM   625  CB  LYS  283      6.624  27.246  68.103  1.00 19.89
ATOM   626  CG  LYS  283      6.596  27.154  69.613  1.00 23.82
ATOM   627  CD  LYS  283      5.948  28.388  70.243  1.00 26.99
ATOM   628  CE  LYS  283      5.645  28.183  71.731  1.00 30.98
ATOM   629  NZ  LYS  283      6.837  27.917  72.599  1.00 34.38
ATOM   630  C   LYS  283      6.873  24.791  67.778  1.00 19.44
ATOM   631  O   LYS  283      7.274  24.120  68.729  1.00 19.31
ATOM   632  N   GLY  284      5.882  24.390  66.983  1.00 19.18
ATOM   633  CA  GLY  284      5.240  23.124  67.254  1.00 18.56
ATOM   634  C   GLY  284      5.981  21.885  66.806  1.00 18.31
ATOM   635  O   GLY  284      5.731  20.805  67.328  1.00 19.56
ATOM   636  N   SER  285      6.941  22.024  65.895  1.00 18.65
ATOM   637  CA  SER  285      7.633  20.844  65.384  1.00 17.51
ATOM   638  CB  SER  285      7.453  20.755  63.870  1.00 19.70
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ATOM	639	OG	SER	285	8.063	21.874	63.212	1.00	18.48
ATOM	640	C	SER	285	9.136	20.728	65.663	1.00	15.25
ATOM	641	O	SER	285	9.705	19.673	65.406	1.00	15.43
ATOM	642	N	TRP	286	9.770	21.759	66.203	1.00	15.99
ATOM	643	CA	TRP	286	11.221	21.642	66.395	1.00	16.28
ATOM	644	CB	TRP	286	11.812	22.920	67.007	1.00	17.10
ATOM	645	CG	TRP	286	11.458	23.226	68.414	1.00	17.32
ATOM	646	CD2	TRP	286	12.117	22.736	69.592	1.00	18.06
ATOM	647	CE2	TRP	286	11.440	23.291	70.709	1.00	20.12
ATOM	648	CE3	TRP	286	13.208	21.882	69.815	1.00	17.92
ATOM	649	CD1	TRP	286	10.445	24.033	68.850	1.00	18.61
ATOM	650	NE1	TRP	286	10.427	24.076	70.227	1.00	18.32
ATOM	651	CZ2	TRP	286	11.816	23.020	72.027	1.00	17.23
ATOM	652	CZ3	TRP	286	13.580	21.608	71.136	1.00	18.42
ATOM	653	CH2	TRP	286	12.889	22.172	72.219	1.00	19.75
ATOM	654	C	TRP	286	11.668	20.443	67.219	1.00	16.59
ATOM	655	O	TRP	286	12.655	19.766	66.886	1.00	17.31
ATOM	656	N	ASN	287	10.938	20.167	68.282	1.00	15.26
ATOM	657	CA	ASN	287	11.301	19.059	69.157	1.00	14.41
ATOM	658	CB	ASN	287	10.508	19.180	70.456	1.00	17.68
ATOM	659	CG	ASN	287	10.894	18.145	71.474	1.00	19.61
ATOM	660	OD1	ASN	287	11.757	18.374	72.348	1.00	23.92
ATOM	661	ND2	ASN	287	10.251	16.991	71.384	1.00	18.83
ATOM	662	C	ASN	287	11.096	17.718	68.448	1.00	14.74
ATOM	663	O	ASN	287	11.954	16.846	68.508	1.00	16.16
ATOM	664	N	GLU	288	9.966	17.555	67.752	1.00	15.22
ATOM	665	CA	GLU	288	9.745	16.319	66.986	1.00	16.77
ATOM	666	CB	GLU	288	8.367	16.358	66.288	1.00	17.55
ATOM	667	CG	GLU	288	7.213	16.044	67.224	1.00	18.68
ATOM	668	CD	GLU	288	5.868	16.134	66.548	1.00	23.02
ATOM	669	OE1	GLU	288	5.786	15.849	65.342	1.00	28.18
ATOM	670	OE2	GLU	288	4.887	16.461	67.243	1.00	29.07
ATOM	671	C	GLU	288	10.838	16.122	65.921	1.00	17.49
ATOM	672	O	GLU	288	11.338	15.014	65.743	1.00	16.93
ATOM	673	N	LEU	289	11.193	17.204	65.220	1.00	14.56
ATOM	674	CA	LEU	289	12.196	17.130	64.173	1.00	15.76

ATOM	675	CB	LEU	289	12.248	18.451	63.390	1.00	14.77
ATOM	676	CG	LEU	289	11.006	18.639	62.483	1.00	16.67
ATOM	677	CD1	LEU	289	10.932	20.093	62.002	1.00	18.25
ATOM	678	CD2	LEU	289	11.083	17.667	61.287	1.00	15.71
ATOM	679	C	LEU	289	13.555	16.784	64.752	1.00	16.05
ATOM	680	O	LEU	289	14.301	16.022	64.138	1.00	16.56
ATOM	681	N	LEU	290	13.884	17.312	65.929	1.00	16.37
ATOM	682	CA	LEU	290	15.190	16.951	66.529	1.00	16.68
ATOM	683	CB	LEU	290	15.477	17.734	67.809	1.00	17.02
ATOM	684	CG	LEU	290	15.786	19.219	67.684	1.00	22.29
ATOM	685	CD1	LEU	290	16.294	19.726	69.046	1.00	23.74
ATOM	686	CD2	LEU	290	16.865	19.454	66.604	1.00	25.08
ATOM	687	C	LEU	290	15.229	15.471	66.868	1.00	16.18
ATOM	688	O	LEU	290	16.214	14.803	66.605	1.00	17.45
ATOM	689	N	LEU	291	14.142	14.958	67.465	1.00	16.16
ATOM	690	CA	LEU	291	14.088	13.553	67.826	1.00	17.64
ATOM	691	CB	LEU	291	12.828	13.289	68.666	1.00	17.32
ATOM	692	CG	LEU	291	12.824	13.961	70.046	1.00	20.40
ATOM	693	CD1	LEU	291	11.405	13.964	70.627	1.00	22.18
ATOM	694	CD2	LEU	291	13.789	13.222	70.971	1.00	23.46
ATOM	695	C	LEU	291	14.087	12.662	66.595	1.00	15.65
ATOM	696	O	LEU	291	14.645	11.569	66.611	1.00	17.39
ATOM	697	N	PHE	292	13.434	13.116	65.520	1.00	14.81
ATOM	698	CA	PHE	292	13.360	12.330	64.311	1.00	15.62
ATOM	699	CB	PHE	292	12.392	12.993	63.314	1.00	16.43
ATOM	700	CG	PHE	292	12.003	12.113	62.167	1.00	16.59
ATOM	701	CD1	PHE	292	11.588	10.812	62.389	1.00	18.96
ATOM	702	CD2	PHE	292	12.002	12.607	60.875	1.00	19.01
ATOM	703	CE1	PHE	292	11.170	10.011	61.332	1.00	20.62
ATOM	704	CE2	PHE	292	11.581	11.805	59.805	1.00	18.46
ATOM	705	CZ	PHE	292	11.166	10.499	60.060	1.00	18.06
ATOM	706	C	PHE	292	14.761	12.191	63.713	1.00	15.70
ATOM	707	O	PHE	292	15.132	11.119	63.236	1.00	15.72
ATOM	708	N	ALA	293	15.526	13.278	63.760	1.00	16.34
ATOM	709	CA	ALA	293	16.906	13.267	63.232	1.00	16.73
ATOM	710	CB	ALA	293	17.464	14.702	63.207	1.00	17.74

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ATOM   711  C   ALA  293     17.802  12.368  64.090  1.00 17.09
ATOM   712  O   ALA  293     18.668  11.654  63.570  1.00 17.27
ATOM   713  N   ILE  294     17.623  12.423  65.407  1.00 16.09
ATOM   714  CA  ILE  294     18.389  11.569  66.312  1.00 16.22
ATOM   715  CB  ILE  294     18.032  11.857  67.768  1.00 15.67
ATOM   716  CG2 ILE  294     18.584  10.765  68.679  1.00 16.66
ATOM   717  CG1 ILE  294     18.615  13.218  68.160  1.00 17.00
ATOM   718  CD1 ILE  294     18.206  13.635  69.535  1.00 20.77
ATOM   719  C   ILE  294     18.070  10.111  65.971  1.00 16.74
ATOM   720  O   ILE  294     18.954   9.296  65.833  1.00 16.38
ATOM   721  N   ALA  295     16.791   9.791  65.774  1.00 16.15
ATOM   722  CA  ALA  295     16.452   8.420  65.424  1.00 16.99
ATOM   723  CB  ALA  295     14.937   8.273  65.332  1.00 16.54
ATOM   724  C   ALA  295     17.083   7.993  64.088  1.00 17.97
ATOM   725  O   ALA  295     17.563   6.870  63.954  1.00 18.01
ATOM   726  N   TRP  296     17.071   8.881  63.102  1.00 18.59
ATOM   727  CA  TRP  296     17.625   8.570  61.782  1.00 18.81
ATOM   728  CB  TRP  296     17.321   9.740  60.835  1.00 20.21
ATOM   729  CG  TRP  296     17.849   9.622  59.451  1.00 22.61
ATOM   730  CD2 TRP  296     17.398   8.716  58.433  1.00 25.62
ATOM   731  CE2 TRP  296     18.125   9.007  57.265  1.00 26.25
ATOM   732  CE3 TRP  296     16.448   7.683  58.402  1.00 25.95
ATOM   733  CD1 TRP  296     18.807  10.403  58.871  1.00 26.23
ATOM   734  NE1 TRP  296     18.975  10.043  57.556  1.00 26.50
ATOM   735  CZ2 TRP  296     17.934   8.297  56.063  1.00 27.77
ATOM   736  CZ3 TRP  296     16.257   6.977  57.206  1.00 27.65
ATOM   737  CH2 TRP  296     16.996   7.289  56.061  1.00 25.35
ATOM   738  C   TRP  296     19.133   8.299  61.878  1.00 19.53
ATOM   739  O   TRP  296     19.647   7.296  61.345  1.00 21.43
ATOM   740  N   ARG  297     19.833   9.147  62.623  1.00 18.58
ATOM   741  CA  ARG  297     21.280   8.974  62.748  1.00 18.22
ATOM   742  CB  ARG  297     21.923  10.208  63.376  1.00 18.92
ATOM   743  CG  ARG  297     21.886  11.465  62.525  1.00 20.63
ATOM   744  CD  ARG  297     22.792  12.530  63.137  1.00 26.15
ATOM   745  NE  ARG  297     22.219  13.002  64.381  1.00 29.32
ATOM   746  CZ  ARG  297     21.393  14.040  64.462  1.00 28.97
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ATOM	747	NH1	ARG	297	21.066	14.720	63.373	1.00	29.81
ATOM	748	NH2	ARG	297	20.872	14.372	65.628	1.00	31.03
ATOM	749	C	ARG	297	21.643	7.776	63.605	1.00	18.87
ATOM	750	O	ARG	297	22.738	7.225	63.473	1.00	19.01
ATOM	751	N	SER	298	20.749	7.404	64.511	1.00	17.52
ATOM	752	CA	SER	298	21.023	6.293	65.414	1.00	18.09
ATOM	753	CB	SER	298	20.134	6.407	66.655	1.00	18.94
ATOM	754	OG	SER	298	20.412	7.606	67.381	1.00	18.16
ATOM	755	C	SER	298	20.865	4.929	64.770	1.00	20.63
ATOM	756	O	SER	298	21.310	3.925	65.336	1.00	24.22
ATOM	757	N	MET	299	20.270	4.868	63.582	1.00	20.01
ATOM	758	CA	MET	299	20.106	3.558	62.953	1.00	22.16
ATOM	759	CB	MET	299	19.367	3.682	61.610	1.00	24.42
ATOM	760	CG	MET	299	17.940	4.159	61.735	1.00	24.29
ATOM	761	SD	MET	299	17.091	4.052	60.130	1.00	31.30
ATOM	762	CE	MET	299	18.221	4.950	59.082	1.00	31.06
ATOM	763	C	MET	299	21.431	2.825	62.725	1.00	25.30
ATOM	764	O	MET	299	21.493	1.600	62.859	1.00	26.84
ATOM	765	N	GLU	300	22.485	3.565	62.414	1.00	28.43
ATOM	766	CA	GLU	300	23.775	2.944	62.117	1.00	32.11
ATOM	767	CB	GLU	300	24.736	3.949	61.472	1.00	34.60
ATOM	768	CG	GLU	300	25.355	4.941	62.420	1.00	40.06
ATOM	769	CD	GLU	300	26.689	5.477	61.910	1.00	43.56
ATOM	770	OE1	GLU	300	27.622	4.666	61.729	1.00	46.83
ATOM	771	OE2	GLU	300	26.812	6.703	61.688	1.00	45.34
ATOM	772	C	GLU	300	24.467	2.304	63.300	1.00	32.94
ATOM	773	O	GLU	300	25.389	1.517	63.123	1.00	32.67
ATOM	774	N	PHE	301	24.033	2.649	64.507	1.00	31.51
ATOM	775	CA	PHE	301	24.632	2.094	65.710	1.00	32.60
ATOM	776	CB	PHE	301	24.822	3.214	66.736	1.00	32.49
ATOM	777	CG	PHE	301	25.879	4.203	66.349	1.00	34.07
ATOM	778	CD1	PHE	301	27.223	3.838	66.358	1.00	33.32
ATOM	779	CD2	PHE	301	25.537	5.483	65.929	1.00	33.10
ATOM	780	CE1	PHE	301	28.207	4.737	65.949	1.00	34.17
ATOM	781	CE2	PHE	301	26.506	6.385	65.519	1.00	34.69
ATOM	782	CZ	PHE	301	27.854	6.008	65.530	1.00	33.21

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ATOM   783  C   PHE  301      23.820   0.940  66.301  1.00 33.77
ATOM   784  O   PHE  301      24.127   0.441  67.377  1.00 34.55
ATOM   785  N   LEU  302      22.780   0.516  65.589  1.00 34.80
ATOM   786  CA  LEU  302      21.966  -0.593  66.045  1.00 36.81
ATOM   787  CB  LEU  302      20.641  -0.645  65.287  1.00 34.98
ATOM   788  CG  LEU  302      19.779   0.596  65.488  1.00 31.61
ATOM   789  CD1 LEU  302      18.551   0.528  64.577  1.00 31.62
ATOM   790  CD2 LEU  302      19.386   0.717  66.955  1.00 31.48
ATOM   791  C   LEU  302      22.744  -1.869  65.775  1.00 40.52
ATOM   792  O   LEU  302      23.333  -2.038  64.701  1.00 40.16
ATOM   793  N   THR  303      22.733  -2.764  66.753  1.00 44.10
ATOM   794  CA  THR  303      23.422  -4.037  66.634  1.00 48.80
ATOM   795  CB  THR  303      23.126  -4.933  67.850  1.00 49.83
ATOM   796  OG1 THR  303      23.211  -4.151  69.050  1.00 51.18
ATOM   797  CG2 THR  303      24.132  -6.076  67.924  1.00 51.25
ATOM   798  C   THR  303      22.932  -4.731  65.368  1.00 50.84
ATOM   799  O   THR  303      21.739  -4.703  65.052  1.00 50.20
ATOM   800  N   ALA  304      23.864  -5.341  64.644  1.00 53.24
ATOM   801  CA  ALA  304      23.538  -6.040  63.410  1.00 55.88
ATOM   802  CB  ALA  304      24.739  -6.867  62.946  1.00 56.05
ATOM   803  C   ALA  304      22.317  -6.942  63.575  1.00 57.61
ATOM   804  O   ALA  304      22.133  -7.583  64.617  1.00 58.45
ATOM   805  N   ALA  305      21.481  -6.972  62.540  1.00 59.51
ATOM   806  CA  ALA  305      20.282  -7.797  62.535  1.00 60.68
ATOM   807  CB  ALA  305      19.548  -7.651  61.205  1.00 60.98
ATOM   808  C   ALA  305      20.714  -9.245  62.744  1.00 61.71
ATOM   809  O   ALA  305      19.925 -10.029  63.319  1.00 62.15
ATOM   810  OXT ALA  305      21.848  -9.572  62.316  1.00 61.88
ATOM   811  CB  ALA  316      17.484 -11.402  70.435  1.00 59.02
ATOM   812  C   ALA  316      15.833  -9.781  71.403  1.00 57.95
ATOM   813  O   ALA  316      15.469  -9.327  70.316  1.00 58.69
ATOM   814  N   ALA  316      15.341 -12.224  71.375  1.00 58.18
ATOM   815  CA  ALA  316      16.413 -11.191  71.510  1.00 58.61
ATOM   816  N   ALA  317      15.747  -9.096  72.539  1.00 56.79
ATOM   817  CA  ALA  317      15.218  -7.739  72.587  1.00 54.70
ATOM   818  CB  ALA  317      13.813  -7.745  73.174  1.00 54.73
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ATOM   819  C   ALA  317      16.142  -6.871  73.437  1.00 52.91
ATOM   820  O   ALA  317      15.697  -5.935  74.111  1.00 53.06
ATOM   821  N   SER  318      17.430  -7.207  73.404  1.00 49.42
ATOM   822  CA  SER  318      18.449  -6.478  74.151  1.00 46.14
ATOM   823  CB  SER  318      19.830  -7.056  73.835  1.00 46.72
ATOM   824  OG  SER  318      20.834  -6.462  74.639  1.00 47.98
ATOM   825  C   SER  318      18.378  -5.009  73.723  1.00 43.02
ATOM   826  O   SER  318      18.543  -4.686  72.541  1.00 44.27
ATOM   827  N   PRO  319      18.122  -4.100  74.676  0.50 41.03    AC1
ATOM   828  CD  PRO  319      17.740  -4.342  76.079  0.50 40.29    AC1
ATOM   829  CA  PRO  319      18.033  -2.672  74.351  0.50 38.31    AC1
ATOM   830  CB  PRO  319      17.690  -2.032  75.694  0.50 38.96    AC1
ATOM   831  CG  PRO  319      16.927  -3.116  76.402  0.50 39.34    AC1
ATOM   832  C   PRO  319      19.310  -2.080  73.756  0.50 35.85    AC1
ATOM   833  O   PRO  319      20.394  -2.240  74.319  0.50 35.73    AC1
ATOM   834  N   PRO  320      19.197  -1.403  72.599  1.00 33.69
ATOM   835  CD  PRO  320      18.041  -1.404  71.692  1.00 32.09
ATOM   836  CA  PRO  320      20.362  -0.784  71.952  1.00 30.83
ATOM   837  CB  PRO  320      19.769  -0.083  70.722  1.00 30.11
ATOM   838  CG  PRO  320      18.279  -0.174  70.892  1.00 32.74
ATOM   839  C   PRO  320      21.008   0.185  72.949  1.00 27.19
ATOM   840  O   PRO  320      20.317   0.824  73.756  1.00 27.36
ATOM   841  N   GLN  321      22.328   0.297  72.890  1.00 25.76
ATOM   842  CA  GLN  321      23.060   1.121  73.847  1.00 25.85
ATOM   843  CB  GLN  321      24.262   0.329  74.357  1.00 29.20
ATOM   844  CG  GLN  321      23.925  -1.090  74.757  1.00 34.12
ATOM   845  CD  GLN  321      23.408  -1.197  76.163  1.00 38.11
ATOM   846  OE1 GLN  321      24.127  -0.916  77.123  1.00 40.85
ATOM   847  NE2 GLN  321      22.150  -1.617  76.302  1.00 40.57
ATOM   848  C   GLN  321      23.546   2.495  73.423  1.00 23.90
ATOM   849  O   GLN  321      23.914   3.297  74.275  1.00 24.18
ATOM   850  N   LEU  322      23.536   2.790  72.128  1.00 22.59
ATOM   851  CA  LEU  322      24.050   4.080  71.666  1.00 21.41
ATOM   852  CB  LEU  322      25.291   3.879  70.775  1.00 22.86
ATOM   853  CG  LEU  322      26.560   3.362  71.432  1.00 25.45
ATOM   854  CD1 LEU  322      27.625   3.130  70.345  1.00 28.06
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ATOM	855	CD2	LEU	322	27.036	4.384	72.497	1.00 24.21
ATOM	856	C	LEU	322	23.079	4.942	70.891	1.00 22.08
ATOM	857	O	LEU	322	22.435	4.478	69.961	1.00 23.11
ATOM	858	N	MET	323	23.003	6.205	71.270	1.00 20.81
ATOM	859	CA	MET	323	22.145	7.157	70.590	1.00 21.91
ATOM	860	CB	MET	323	21.213	7.835	71.598	1.00 23.20
ATOM	861	CG	MET	323	20.325	8.922	70.978	1.00 22.36
ATOM	862	SD	MET	323	19.196	9.636	72.187	1.00 22.04
ATOM	863	CE	MET	323	18.026	8.314	72.302	1.00 22.12
ATOM	864	C	MET	323	23.054	8.187	69.914	1.00 25.54
ATOM	865	O	MET	323	24.002	8.691	70.530	1.00 25.31
ATOM	866	N	CYS	324	22.781	8.506	68.650	1.00 22.41
ATOM	867	CA	CYS	324	23.619	9.483	67.941	1.00 24.83
ATOM	868	CB	CYS	324	23.854	9.029	66.512	1.00 23.91
ATOM	869	SG	CYS	324	24.921	10.185	65.588	1.00 27.74
ATOM	870	C	CYS	324	22.995	10.873	67.950	1.00 24.34
ATOM	871	O	CYS	324	22.010	11.148	67.249	1.00 24.90
ATOM	872	N	LEU	325	23.560	11.758	68.749	1.00 24.49
ATOM	873	CA	LEU	325	23.038	13.114	68.843	1.00 25.66
ATOM	874	CB	LEU	325	23.421	13.746	70.183	1.00 26.79
ATOM	875	CG	LEU	325	22.935	12.964	71.421	1.00 27.19
ATOM	876	CD1	LEU	325	23.256	13.744	72.704	1.00 29.28
ATOM	877	CD2	LEU	325	21.423	12.732	71.320	1.00 27.92
ATOM	878	C	LEU	325	23.513	13.990	67.682	1.00 28.10
ATOM	879	O	LEU	325	22.860	14.978	67.344	1.00 31.20
ATOM	880	N	MET	326	24.650	13.618	67.094	1.00 28.83
ATOM	881	CA	MET	326	25.253	14.311	65.947	1.00 30.95
ATOM	882	CB	MET	326	25.726	15.721	66.350	1.00 31.86
ATOM	883	CG	MET	326	26.894	15.710	67.335	1.00 31.84
ATOM	884	SD	MET	326	27.648	17.333	67.693	1.00 34.98
ATOM	885	CE	MET	326	29.085	16.800	68.706	1.00 30.77
ATOM	886	C	MET	326	26.462	13.453	65.513	1.00 33.06
ATOM	887	O	MET	326	26.882	12.565	66.242	1.00 32.71
ATOM	888	N	PRO	327	27.013	13.682	64.307	1.00 35.54
ATOM	889	CD	PRO	327	26.511	14.545	63.227	1.00 35.87
ATOM	890	CA	PRO	327	28.180	12.896	63.857	1.00 36.24

ATOM	891	CB	PRO	327	28.508	13.519	62.503	1.00	37.87
ATOM	892	CG	PRO	327	27.159	13.932	62.001	1.00	35.11
ATOM	893	C	PRO	327	29.353	13.035	64.836	1.00	38.75
ATOM	894	O	PRO	327	29.754	14.154	65.155	1.00	38.99
ATOM	895	N	GLY	328	29.890	11.908	65.314	1.00	38.52
ATOM	896	CA	GLY	328	31.001	11.933	66.257	1.00	38.65
ATOM	897	C	GLY	328	30.606	12.217	67.700	1.00	38.39
ATOM	898	O	GLY	328	31.431	12.604	68.545	1.00	39.05
ATOM	899	N	MET	329	29.326	12.020	67.994	1.00	36.32
ATOM	900	CA	MET	329	28.830	12.251	69.326	1.00	34.24
ATOM	901	CB	MET	329	28.343	13.693	69.451	1.00	38.91
ATOM	902	CG	MET	329	27.462	13.991	70.649	1.00	44.24
ATOM	903	SD	MET	329	28.233	13.696	72.235	1.00	50.95
ATOM	904	CE	MET	329	26.854	12.835	73.089	1.00	48.58
ATOM	905	C	MET	329	27.700	11.271	69.603	1.00	30.52
ATOM	906	O	MET	329	26.647	11.331	68.975	1.00	28.92
ATOM	907	N	THR	330	27.960	10.324	70.490	1.00	26.42
ATOM	908	CA	THR	330	26.933	9.370	70.865	1.00	23.65
ATOM	909	CB	THR	330	27.338	7.895	70.542	1.00	24.12
ATOM	910	OG1	THR	330	28.672	7.654	71.005	1.00	27.18
ATOM	911	CG2	THR	330	27.269	7.622	69.034	1.00	26.34
ATOM	912	C	THR	330	26.685	9.475	72.360	1.00	23.23
ATOM	913	O	THR	330	27.572	9.802	73.146	1.00	23.91
ATOM	914	N	LEU	331	25.450	9.211	72.748	1.00	20.37
ATOM	915	CA	LEU	331	25.082	9.213	74.142	1.00	21.33
ATOM	916	CB	LEU	331	23.773	9.986	74.340	1.00	24.38
ATOM	917	CG	LEU	331	23.113	9.731	75.696	1.00	25.70
ATOM	918	CD1	LEU	331	23.979	10.317	76.825	1.00	30.48
ATOM	919	CD2	LEU	331	21.723	10.348	75.694	1.00	29.64
ATOM	920	C	LEU	331	24.892	7.737	74.489	1.00	21.13
ATOM	921	O	LEU	331	24.158	7.026	73.819	1.00	19.21
ATOM	922	N	HIS	332	25.582	7.262	75.525	1.00	18.80
ATOM	923	CA	HIS	332	25.472	5.864	75.901	1.00	18.64
ATOM	924	CB	HIS	332	26.740	5.417	76.658	1.00	18.77
ATOM	925	CG	HIS	332	26.826	3.938	76.862	1.00	21.68
ATOM	926	CD2	HIS	332	27.533	2.991	76.205	1.00	22.97

ATOM 927 ND1 HIS 332 26.092 3.273 77.824 1.00 22.38
ATOM 928 CE1 HIS 332 26.340 1.978 77.745 1.00 23.74
ATOM 929 NE2 HIS 332 27.213 1.778 76.769 1.00 25.26
ATOM 930 C HIS 332 24.262 5.721 76.820 1.00 18.95
ATOM 931 O HIS 332 23.981 6.620 77.616 1.00 19.91
ATOM 932 N ARG 333 23.594 4.581 76.715 1.00 19.39
ATOM 933 CA ARG 333 22.394 4.282 77.509 1.00 19.71
ATOM 934 CB ARG 333 21.930 2.850 77.235 1.00 20.65
ATOM 935 CG ARG 333 20.582 2.512 77.896 1.00 21.54
ATOM 936 CD ARG 333 20.018 1.212 77.353 1.00 21.69
ATOM 937 NE ARG 333 18.703 0.862 77.899 1.00 20.98
ATOM 938 CZ ARG 333 18.501 0.034 78.921 1.00 22.46
ATOM 939 NH1 ARG 333 19.535 -0.547 79.531 1.00 24.12
ATOM 940 NH2 ARG 333 17.255 -0.241 79.309 1.00 20.87
ATOM 941 C ARG 333 22.643 4.463 79.018 1.00 21.14
ATOM 942 O ARG 333 21.782 4.926 79.755 1.00 18.39
ATOM 943 N ASN 334 23.832 4.107 79.484 1.00 21.27
ATOM 944 CA ASN 334 24.114 4.259 80.910 1.00 23.47
ATOM 945 CB ASN 334 25.486 3.653 81.244 1.00 24.93
ATOM 946 CG ASN 334 25.504 2.119 81.158 1.00 25.59
ATOM 947 OD1 ASN 334 24.467 1.461 81.054 1.00 26.24
ATOM 948 ND2 ASN 334 26.707 1.544 81.204 1.00 29.08
ATOM 949 C ASN 334 24.048 5.718 81.380 1.00 22.91
ATOM 950 O ASN 334 23.649 6.000 82.530 1.00 22.99
ATOM 951 N SER 335 24.441 6.657 80.524 1.00 22.89
ATOM 952 CA SER 335 24.378 8.059 80.904 1.00 22.41
ATOM 953 CB SER 335 25.178 8.915 79.930 1.00 27.35
ATOM 954 OG SER 335 26.517 8.437 79.856 1.00 31.39
ATOM 955 C SER 335 22.908 8.484 80.939 1.00 23.03
ATOM 956 O SER 335 22.496 9.260 81.809 1.00 22.21
ATOM 957 N ALA 336 22.126 7.970 79.989 1.00 21.81
ATOM 958 CA ALA 336 20.703 8.255 79.952 1.00 21.09
ATOM 959 CB ALA 336 20.060 7.595 78.718 1.00 21.81
ATOM 960 C ALA 336 20.044 7.744 81.232 1.00 21.37
ATOM 961 O ALA 336 19.209 8.425 81.830 1.00 19.40
ATOM 962 N LEU 337 20.423 6.540 81.660 1.00 19.77

ATOM	963	CA	LEU	337	19.860	5.960	82.865	1.00	19.59
ATOM	964	CB	LEU	337	20.374	4.517	83.039	1.00	19.20
ATOM	965	CG	LEU	337	19.835	3.502	82.031	1.00	20.97
ATOM	966	CD1	LEU	337	20.702	2.280	82.055	1.00	23.49
ATOM	967	CD2	LEU	337	18.391	3.164	82.329	1.00	21.07
ATOM	968	C	LEU	337	20.206	6.777	84.089	1.00	20.54
ATOM	969	O	LEU	337	19.364	6.997	84.985	1.00	19.57
ATOM	970	N	GLN	338	21.454	7.226	84.131	1.00	21.36
ATOM	971	CA	GLN	338	21.920	7.994	85.264	1.00	22.39
ATOM	972	CB	GLN	338	23.439	8.206	85.179	1.00	22.44
ATOM	973	CG	GLN	338	23.973	8.755	86.488	1.00	27.14
ATOM	974	CD	GLN	338	25.467	9.026	86.481	1.00	29.23
ATOM	975	OE1	GLN	338	25.955	9.827	87.278	1.00	30.73
ATOM	976	NE2	GLN	338	26.196	8.360	85.596	1.00	30.79
ATOM	977	C	GLN	338	21.200	9.331	85.381	1.00	23.40
ATOM	978	O	GLN	338	20.894	9.790	86.490	1.00	21.75
ATOM	979	N	ALA	339	20.899	9.935	84.227	1.00	22.63
ATOM	980	CA	ALA	339	20.215	11.217	84.191	1.00	24.41
ATOM	981	CB	ALA	339	20.430	11.903	82.832	1.00	23.46
ATOM	982	C	ALA	339	18.727	11.082	84.463	1.00	24.73
ATOM	983	O	ALA	339	18.059	12.084	84.641	1.00	27.16
ATOM	984	N	GLY	340	18.218	9.850	84.499	1.00	22.58
ATOM	985	CA	GLY	340	16.803	9.622	84.754	1.00	23.89
ATOM	986	C	GLY	340	15.898	9.580	83.531	1.00	25.09
ATOM	987	O	GLY	340	14.666	9.607	83.666	1.00	25.54
ATOM	988	N	VAL	341	16.492	9.479	82.346	1.00	23.51
ATOM	989	CA	VAL	341	15.719	9.473	81.095	1.00	20.92
ATOM	990	CB	VAL	341	16.134	10.677	80.211	1.00	21.83
ATOM	991	CG1	VAL	341	15.838	11.981	80.942	1.00	21.94
ATOM	992	CG2	VAL	341	17.621	10.577	79.858	1.00	21.91
ATOM	993	C	VAL	341	15.891	8.185	80.300	1.00	20.24
ATOM	994	O	VAL	341	15.803	8.182	79.083	1.00	19.53
ATOM	995	N	GLY	342	16.132	7.079	80.999	1.00	19.65
ATOM	996	CA	GLY	342	16.324	5.827	80.301	1.00	18.76
ATOM	997	C	GLY	342	15.104	5.352	79.541	1.00	19.27
ATOM	998	O	GLY	342	15.230	4.771	78.470	1.00	18.82

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ATOM   999 N   GLN 343    13.922  5.598 80.088 0.50 18.31    AC1
ATOM  1000 CA  GLN 343    12.706  5.163 79.422 0.50 19.11    AC1
ATOM  1001 CB  GLN 343    11.507  5.485 80.305 0.50 19.94    AC1
ATOM  1002 CG  GLN 343    10.200  4.866 79.867 0.50 22.91    AC1
ATOM  1003 CD  GLN 343     9.082  5.177 80.852 0.50 24.13    AC1
ATOM  1004 OE1 GLN 343     8.669  6.326 80.995 0.50 26.85    AC1
ATOM  1005 NE2 GLN 343     8.606  4.154 81.555 0.50 25.40    AC1
ATOM  1006 C   GLN 343    12.542  5.813 78.043 0.50 19.14    AC1
ATOM  1007 O   GLN 343    12.318  5.127 77.050 0.50 18.83    AC1
ATOM  1008 N   ILE 344    12.664  7.136 77.977 1.00 17.95
ATOM  1009 CA  ILE 344    12.506  7.812 76.693 1.00 17.74
ATOM  1010 CB  ILE 344    12.348  9.372 76.875 1.00 18.47
ATOM  1011 CG2 ILE 344    13.700 10.010 77.231 1.00 20.66
ATOM  1012 CG1 ILE 344    11.754  9.984 75.596 1.00 19.04
ATOM  1013 CD1 ILE 344    11.445 11.499 75.662 1.00 21.07
ATOM  1014 C   ILE 344    13.641  7.448 75.718 1.00 17.34
ATOM  1015 O   ILE 344    13.440  7.389 74.499 1.00 16.12
ATOM  1016 N   PHE 345    14.844  7.210 76.248 1.00 16.60
ATOM  1017 CA  PHE 345    15.976  6.826 75.417 1.00 17.63
ATOM  1018 CB  PHE 345    17.208  6.636 76.322 1.00 17.86
ATOM  1019 CG  PHE 345    18.455  6.189 75.613 1.00 18.24
ATOM  1020 CD1 PHE 345    18.657  4.848 75.273 1.00 18.20
ATOM  1021 CD2 PHE 345    19.470  7.090 75.363 1.00 20.10
ATOM  1022 CE1 PHE 345    19.854  4.412 74.706 1.00 19.01
ATOM  1023 CE2 PHE 345    20.663  6.673 74.798 1.00 17.96
ATOM  1024 CZ  PHE 345    20.861  5.328 74.469 1.00 18.58
ATOM  1025 C   PHE 345    15.603  5.522 74.710 1.00 18.98
ATOM  1026 O   PHE 345    15.756  5.389 73.491 1.00 18.15
ATOM  1027 N   ASP 346    15.072  4.568 75.480 1.00 18.04
ATOM  1028 CA  ASP 346    14.695  3.300 74.894 1.00 18.83
ATOM  1029 CB  ASP 346    14.285  2.302 75.988 1.00 19.96
ATOM  1030 CG  ASP 346    15.467  1.768 76.786 1.00 24.04
ATOM  1031 OD1 ASP 346    16.630  2.038 76.430 1.00 24.95
ATOM  1032 OD2 ASP 346    15.232  1.043 77.784 1.00 24.86
ATOM  1033 C   ASP 346    13.550  3.462 73.872 1.00 18.04
ATOM  1034 O   ASP 346    13.549  2.782 72.841 1.00 19.39
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ATOM	1035	N	ARG	347	12.603	4.359	74.138	1.00	19.77
ATOM	1036	CA	ARG	347	11.493	4.579	73.188	1.00	20.42
ATOM	1037	CB	ARG	347	10.443	5.558	73.708	1.00	24.20
ATOM	1038	CG	ARG	347	9.527	5.024	74.786	1.00	26.30
ATOM	1039	CD	ARG	347	8.310	5.929	74.937	1.00	28.76
ATOM	1040	NE	ARG	347	7.383	5.807	73.813	1.00	29.58
ATOM	1041	CZ	ARG	347	6.312	6.577	73.629	1.00	31.91
ATOM	1042	NH1	ARG	347	6.028	7.536	74.492	1.00	32.14
ATOM	1043	NH2	ARG	347	5.522	6.378	72.579	1.00	32.47
ATOM	1044	C	ARG	347	12.012	5.120	71.875	1.00	20.09
ATOM	1045	O	ARG	347	11.586	4.703	70.806	1.00	18.14
ATOM	1046	N	VAL	348	12.939	6.073	71.945	1.00	18.48
ATOM	1047	CA	VAL	348	13.480	6.621	70.708	1.00	18.94
ATOM	1048	CB	VAL	348	14.532	7.713	70.991	1.00	18.19
ATOM	1049	CG1	VAL	348	15.286	8.052	69.706	1.00	18.18
ATOM	1050	CG2	VAL	348	13.862	8.930	71.600	1.00	19.11
ATOM	1051	C	VAL	348	14.143	5.518	69.882	1.00	18.63
ATOM	1052	O	VAL	348	13.885	5.380	68.691	1.00	17.99
ATOM	1053	N	LEU	349	14.981	4.709	70.514	1.00	18.35
ATOM	1054	CA	LEU	349	15.679	3.686	69.749	1.00	19.38
ATOM	1055	CB	LEU	349	16.906	3.175	70.526	1.00	20.34
ATOM	1056	CG	LEU	349	17.920	4.286	70.807	1.00	20.49
ATOM	1057	CD1	LEU	349	19.173	3.626	71.408	1.00	23.32
ATOM	1058	CD2	LEU	349	18.273	5.078	69.500	1.00	18.92
ATOM	1059	C	LEU	349	14.822	2.509	69.294	1.00	20.39
ATOM	1060	O	LEU	349	15.112	1.901	68.263	1.00	19.62
ATOM	1061	N	SER	350	13.746	2.208	70.025	1.00	21.15
ATOM	1062	CA	SER	350	12.907	1.074	69.623	1.00	23.27
ATOM	1063	CB	SER	350	12.443	0.294	70.855	1.00	25.65
ATOM	1064	OG	SER	350	11.622	1.081	71.687	1.00	28.64
ATOM	1065	C	SER	350	11.698	1.451	68.766	1.00	21.84
ATOM	1066	O	SER	350	11.424	0.790	67.762	1.00	25.35
ATOM	1067	N	GLU	351	10.986	2.516	69.131	1.00	22.62
ATOM	1068	CA	GLU	351	9.801	2.906	68.368	1.00	22.04
ATOM	1069	CB	GLU	351	8.834	3.680	69.252	1.00	22.43
ATOM	1070	CG	GLU	351	8.454	2.916	70.486	1.00	26.86

ATOM	1071	CD	GLU	351	7.434	3.650	71.303	1.00	28.97	
ATOM	1072	OE1	GLU	351	7.473	3.544	72.548	1.00	31.85	
ATOM	1073	OE2	GLU	351	6.581	4.330	70.691	1.00	32.68	
ATOM	1074	C	GLU	351	10.133	3.708	67.132	1.00	22.11	
ATOM	1075	O	GLU	351	9.348	3.766	66.183	1.00	22.30	
ATOM	1076	N	LEU	352	11.309	4.328	67.113	1.00	19.99	
ATOM	1077	CA	LEU	352	11.696	5.083	65.934	1.00	19.01	
ATOM	1078	CB	LEU	352	12.043	6.555	66.293	1.00	18.64	
ATOM	1079	CG	LEU	352	10.911	7.365	66.950	1.00	19.12	
ATOM	1080	CD1	LEU	352	11.445	8.742	67.339	1.00	19.51	
ATOM	1081	CD2	LEU	352	9.703	7.505	66.018	1.00	19.25	
ATOM	1082	C	LEU	352	12.859	4.467	65.163	1.00	19.51	
ATOM	1083	O	LEU	352	12.704	3.977	64.038	1.00	21.10	
ATOM	1084	N	SER	353	14.052	4.464	65.754	0.50	18.72	AC1
ATOM	1085	CA	SER	353	15.203	3.933	65.034	0.50	18.55	AC1
ATOM	1086	CB	SER	353	16.473	4.032	65.883	0.50	16.66	AC1
ATOM	1087	OG	SER	353	16.782	5.378	66.160	0.50	11.47	AC1
ATOM	1088	C	SER	353	15.045	2.500	64.546	0.50	19.60	AC1
ATOM	1089	O	SER	353	15.207	2.236	63.355	0.50	20.26	AC1
ATOM	1090	N	LEU	354	14.746	1.579	65.455	1.00	21.67	
ATOM	1091	CA	LEU	354	14.602	0.181	65.051	1.00	23.55	
ATOM	1092	CB	LEU	354	14.360	-0.715	66.278	1.00	24.35	
ATOM	1093	CG	LEU	354	14.284	-2.222	66.012	1.00	30.18	
ATOM	1094	CD1	LEU	354	15.388	-2.664	65.055	1.00	31.88	
ATOM	1095	CD2	LEU	354	14.392	-2.944	67.345	1.00	31.36	
ATOM	1096	C	LEU	354	13.489	-0.011	64.009	1.00	24.82	
ATOM	1097	O	LEU	354	13.696	-0.684	63.004	1.00	25.66	
ATOM	1098	N	LYS	355	12.324	0.587	64.234	1.00	26.97	
ATOM	1099	CA	LYS	355	11.236	0.454	63.272	1.00	26.95	
ATOM	1100	CB	LYS	355	10.003	1.226	63.735	1.00	29.30	
ATOM	1101	CG	LYS	355	9.228	0.572	64.843	1.00	34.34	
ATOM	1102	CD	LYS	355	8.440	-0.616	64.321	1.00	38.57	
ATOM	1103	CE	LYS	355	7.365	-1.007	65.319	1.00	39.54	
ATOM	1104	NZ	LYS	355	7.883	-0.958	66.713	1.00	40.20	
ATOM	1105	C	LYS	355	11.637	0.964	61.899	1.00	27.30	
ATOM	1106	O	LYS	355	11.281	0.369	60.883	1.00	28.58	

ATOM	1107	N	MET	356	12.362	2.080	61.860	1.00	25.41
ATOM	1108	CA	MET	356	12.787	2.641	60.594	1.00	25.37
ATOM	1109	CB	MET	356	13.279	4.071	60.778	1.00	27.04
ATOM	1110	CG	MET	356	12.126	5.017	60.918	1.00	26.57
ATOM	1111	SD	MET	356	12.669	6.671	60.768	1.00	36.72
ATOM	1112	CE	MET	356	13.015	6.835	62.357	1.00	16.80
ATOM	1113	C	MET	356	13.836	1.808	59.896	1.00	26.93
ATOM	1114	O	MET	356	13.907	1.807	58.676	1.00	25.41
ATOM	1115	N	ARG	357	14.672	1.114	60.661	1.00	27.88
ATOM	1116	CA	ARG	357	15.656	0.281	60.003	1.00	29.75
ATOM	1117	CB	ARG	357	16.733	-0.214	60.961	1.00	31.09
ATOM	1118	CG	ARG	357	17.748	-1.056	60.213	1.00	35.17
ATOM	1119	CD	ARG	357	18.840	-1.607	61.112	1.00	38.46
ATOM	1120	NE	ARG	357	18.313	-2.543	62.097	1.00	41.53
ATOM	1121	CZ	ARG	357	19.066	-3.164	63.003	1.00	43.38
ATOM	1122	NH1	ARG	357	20.376	-2.942	63.037	1.00	42.92
ATOM	1123	NH2	ARG	357	18.512	-3.995	63.879	1.00	43.48
ATOM	1124	C	ARG	357	14.926	-0.925	59.422	1.00	29.63
ATOM	1125	O	ARG	357	15.218	-1.353	58.310	1.00	29.83
ATOM	1126	N	THR	358	13.966	-1.452	60.171	1.00	29.51
ATOM	1127	CA	THR	358	13.204	-2.609	59.704	1.00	30.65
ATOM	1128	CB	THR	358	12.273	-3.117	60.812	1.00	31.00
ATOM	1129	OG1	THR	358	13.071	-3.609	61.895	1.00	32.46
ATOM	1130	CG2	THR	358	11.374	-4.260	60.306	1.00	34.28
ATOM	1131	C	THR	358	12.408	-2.281	58.438	1.00	30.73
ATOM	1132	O	THR	358	12.286	-3.114	57.533	1.00	32.33
ATOM	1133	N	LEU	359	11.895	-1.056	58.359	1.00	29.40
ATOM	1134	CA	LEU	359	11.124	-0.610	57.201	1.00	29.68
ATOM	1135	CB	LEU	359	10.242	0.583	57.605	1.00	30.32
ATOM	1136	CG	LEU	359	8.732	0.609	57.321	1.00	34.26
ATOM	1137	CD1	LEU	359	8.197	2.038	57.529	1.00	33.77
ATOM	1138	CD2	LEU	359	8.452	0.142	55.900	1.00	34.08
ATOM	1139	C	LEU	359	12.046	-0.168	56.066	1.00	28.77
ATOM	1140	O	LEU	359	11.585	0.164	54.974	1.00	27.98
ATOM	1141	N	ARG	360	13.349	-0.130	56.327	1.00	30.53
ATOM	1142	CA	ARG	360	14.315	0.310	55.327	1.00	30.15

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ATOM  1143  CB  ARG  360      14.381  -0.695  54.178  1.00 33.80
ATOM  1144  CG  ARG  360      14.798  -2.076  54.625  1.00 36.43
ATOM  1145  CD  ARG  360      14.018  -3.165  53.900  1.00 39.56
ATOM  1146  NE  ARG  360      12.588  -3.168  54.226  1.00 41.14
ATOM  1147  CZ  ARG  360      11.618  -2.942  53.340  1.00 42.18
ATOM  1148  NH1 ARG  360      11.918  -2.688  52.071  1.00 41.02
ATOM  1149  NH2 ARG  360      10.345  -2.983  53.717  1.00 42.86
ATOM  1150  C   ARG  360      13.975   1.699  54.787  1.00 29.92
ATOM  1151  O   ARG  360      14.073   1.958  53.592  1.00 28.84
ATOM  1152  N   VAL  361      13.569   2.600  55.677  1.00 27.64
ATOM  1153  CA  VAL  361      13.261   3.956  55.267  1.00 25.17
ATOM  1154  CB  VAL  361      12.909   4.819  56.480  1.00 24.00
ATOM  1155  CG1 VAL  361      12.684   6.254  56.066  1.00 24.37
ATOM  1156  CG2 VAL  361      11.688   4.249  57.166  1.00 23.19
ATOM  1157  C   VAL  361      14.504   4.525  54.594  1.00 25.34
ATOM  1158  O   VAL  361      15.613   4.407  55.133  1.00 25.79
ATOM  1159  N   ASP  362      14.344   5.109  53.404  1.00 24.62
ATOM  1160  CA  ASP  362      15.481   5.712  52.718  1.00 24.80
ATOM  1161  CB  ASP  362      15.540   5.316  51.223  1.00 27.01
ATOM  1162  CG  ASP  362      14.307   5.720  50.433  1.00 29.25
ATOM  1163  OD1 ASP  362      13.697   6.764  50.731  1.00 27.58
ATOM  1164  OD2 ASP  362      13.963   4.987  49.479  1.00 32.41
ATOM  1165  C   ASP  362      15.520   7.226  52.863  1.00 25.99
ATOM  1166  O   ASP  362      14.631   7.823  53.486  1.00 25.65
ATOM  1167  N   GLN  363      16.561   7.845  52.312  1.00 24.73
ATOM  1168  CA  GLN  363      16.742   9.286  52.405  1.00 26.50
ATOM  1169  CB  GLN  363      18.044   9.682  51.690  1.00 31.84
ATOM  1170  CG  GLN  363      18.339  11.179  51.662  1.00 36.89
ATOM  1171  CD  GLN  363      19.008  11.689  52.921  1.00 40.13
ATOM  1172  OE1 GLN  363      18.615  11.346  54.047  1.00 42.87
ATOM  1173  NE2 GLN  363      20.013  12.536  52.743  1.00 40.44
ATOM  1174  C   GLN  363      15.540  10.070  51.855  1.00 25.17
ATOM  1175  O   GLN  363      15.077  11.020  52.480  1.00 22.69
ATOM  1176  N   ALA  364      15.023   9.659  50.701  1.00 24.53
ATOM  1177  CA  ALA  364      13.863  10.340  50.099  1.00 22.80
ATOM  1178  CB  ALA  364      13.524   9.691  48.753  1.00 22.91
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ATOM  1179  C   ALA  364     12.631  10.326  51.022  1.00 21.81
ATOM  1180  O   ALA  364     11.946  11.336  51.178  1.00 21.88
ATOM  1181  N   GLU  365     12.362   9.188  51.636  1.00 22.72
ATOM  1182  CA  GLU  365     11.218   9.062  52.532  1.00 21.63
ATOM  1183  CB  GLU  365     10.990   7.585  52.856  1.00 22.68
ATOM  1184  CG  GLU  365     10.724   6.806  51.583  1.00 23.15
ATOM  1185  CD  GLU  365     10.797   5.303  51.723  1.00 28.04
ATOM  1186  OE1 GLU  365     11.632   4.813  52.501  1.00 26.39
ATOM  1187  OE2 GLU  365     10.034   4.607  51.010  1.00 27.63
ATOM  1188  C   GLU  365     11.454   9.881  53.798  1.00 22.43
ATOM  1189  O   GLU  365     10.557  10.570  54.298  1.00 22.18
ATOM  1190  N   TYR  366     12.681   9.822  54.304  1.00 22.10
ATOM  1191  CA  TYR  366     13.026  10.580  55.506  1.00 22.15
ATOM  1192  CB  TYR  366     14.494  10.316  55.871  1.00 22.04
ATOM  1193  CG  TYR  366     15.010  11.209  56.986  1.00 22.63
ATOM  1194  CD1 TYR  366     14.580  11.030  58.307  1.00 21.87
ATOM  1195  CE1 TYR  366     15.023  11.864  59.328  1.00 22.24
ATOM  1196  CD2 TYR  366     15.903  12.246  56.715  1.00 20.88
ATOM  1197  CE2 TYR  366     16.366  13.092  57.731  1.00 22.98
ATOM  1198  CZ  TYR  366     15.913  12.899  59.041  1.00 22.25
ATOM  1199  OH  TYR  366     16.315  13.752  60.054  1.00 23.04
ATOM  1200  C   TYR  366     12.797  12.095  55.332  1.00 19.98
ATOM  1201  O   TYR  366     12.209  12.731  56.199  1.00 19.55
ATOM  1202  N   VAL  367     13.260  12.676  54.225  1.00 20.09
ATOM  1203  CA  VAL  367     13.080  14.106  54.034  1.00 19.12
ATOM  1204  CB  VAL  367     13.955  14.666  52.891  1.00 20.38
ATOM  1205  CG1 VAL  367     15.446  14.473  53.249  1.00 21.37
ATOM  1206  CG2 VAL  367     13.609  14.009  51.554  1.00 19.90
ATOM  1207  C   VAL  367     11.607  14.458  53.784  1.00 18.65
ATOM  1208  O   VAL  367     11.165  15.538  54.178  1.00 18.48
ATOM  1209  N   ALA  368     10.868  13.552  53.147  1.00 20.47
ATOM  1210  CA  ALA  368      9.447  13.787  52.893  1.00 19.05
ATOM  1211  CB  ALA  368      8.854  12.668  51.988  1.00 18.93
ATOM  1212  C   ALA  368      8.714  13.813  54.240  1.00 19.17
ATOM  1213  O   ALA  368      7.863  14.682  54.487  1.00 18.81
ATOM  1214  N   LEU  369      9.048  12.871  55.112  1.00 19.43
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ATOM	1215	CA	LEU	369	8.417	12.819	56.428	1.00	17.85
ATOM	1216	CB	LEU	369	8.807	11.526	57.147	1.00	20.14
ATOM	1217	CG	LEU	369	8.153	10.250	56.565	1.00	21.25
ATOM	1218	CD1	LEU	369	8.810	9.041	57.154	1.00	22.02
ATOM	1219	CD2	LEU	369	6.626	10.219	56.856	1.00	21.64
ATOM	1220	C	LEU	369	8.772	14.076	57.235	1.00	19.07
ATOM	1221	O	LEU	369	7.945	14.606	57.965	1.00	17.17
ATOM	1222	N	LYS	370	10.007	14.567	57.120	1.00	18.01
ATOM	1223	CA	LYS	370	10.363	15.799	57.826	1.00	19.26
ATOM	1224	CB	LYS	370	11.819	16.199	57.522	1.00	18.97
ATOM	1225	CG	LYS	370	12.888	15.349	58.203	1.00	21.31
ATOM	1226	CD	LYS	370	14.304	15.860	57.845	1.00	25.49
ATOM	1227	CE	LYS	370	14.445	17.367	58.009	1.00	25.79
ATOM	1228	NZ	LYS	370	15.878	17.841	57.879	1.00	29.87
ATOM	1229	C	LYS	370	9.440	16.949	57.388	1.00	17.68
ATOM	1230	O	LYS	370	8.950	17.717	58.203	1.00	17.05
ATOM	1231	N	ALA	371	9.209	17.075	56.081	1.00	17.98
ATOM	1232	CA	ALA	371	8.368	18.154	55.596	1.00	17.26
ATOM	1233	CB	ALA	371	8.344	18.154	54.065	1.00	19.00
ATOM	1234	C	ALA	371	6.957	17.957	56.140	1.00	15.65
ATOM	1235	O	ALA	371	6.299	18.909	56.533	1.00	17.13
ATOM	1236	N	ILE	372	6.492	16.713	56.151	1.00	14.92
ATOM	1237	CA	ILE	372	5.146	16.450	56.673	1.00	16.38
ATOM	1238	CB	ILE	372	4.743	14.956	56.430	1.00	15.28
ATOM	1239	CG2	ILE	372	3.477	14.602	57.245	1.00	17.98
ATOM	1240	CG1	ILE	372	4.566	14.730	54.915	1.00	18.14
ATOM	1241	CD1	ILE	372	4.413	13.271	54.530	1.00	18.13
ATOM	1242	C	ILE	372	5.038	16.795	58.163	1.00	16.98
ATOM	1243	O	ILE	372	4.028	17.317	58.606	1.00	16.87
ATOM	1244	N	ILE	373	6.089	16.522	58.942	1.00	14.47
ATOM	1245	CA	ILE	373	6.080	16.829	60.369	1.00	15.13
ATOM	1246	CB	ILE	373	7.392	16.251	61.042	1.00	13.81
ATOM	1247	CG2	ILE	373	7.530	16.783	62.463	1.00	15.08
ATOM	1248	CG1	ILE	373	7.340	14.717	61.052	1.00	14.66
ATOM	1249	CD1	ILE	373	8.709	14.031	61.219	1.00	17.60
ATOM	1250	C	ILE	373	5.962	18.350	60.604	1.00	15.01

ATOM 1251 O ILE 373 5.212 18.817 61.477 1.00 15.67
ATOM 1252 N LEU 374 6.702 19.109 59.796 1.00 16.23
ATOM 1253 CA LEU 374 6.688 20.557 59.880 1.00 15.91
ATOM 1254 CB LEU 374 7.738 21.160 58.942 1.00 18.27
ATOM 1255 CG LEU 374 7.702 22.700 58.759 1.00 19.49
ATOM 1256 CD1 LEU 374 8.184 23.403 60.044 1.00 18.70
ATOM 1257 CD2 LEU 374 8.596 23.092 57.597 1.00 19.61
ATOM 1258 C LEU 374 5.316 21.128 59.490 1.00 17.14
ATOM 1259 O LEU 374 4.765 21.980 60.167 1.00 16.72
ATOM 1260 N LEU 375 4.803 20.662 58.367 1.00 17.78
ATOM 1261 CA LEU 375 3.561 21.202 57.831 1.00 17.01
ATOM 1262 CB LEU 375 3.573 21.071 56.301 1.00 19.06
ATOM 1263 CG LEU 375 4.788 21.715 55.581 1.00 18.84
ATOM 1264 CD1 LEU 375 4.903 21.197 54.151 1.00 18.22
ATOM 1265 CD2 LEU 375 4.644 23.234 55.610 1.00 19.41
ATOM 1266 C LEU 375 2.349 20.514 58.422 1.00 19.26
ATOM 1267 O LEU 375 1.603 19.823 57.705 1.00 19.50
ATOM 1268 N ASN 376 2.178 20.727 59.723 1.00 16.95
ATOM 1269 CA ASN 376 1.087 20.136 60.510 1.00 19.78
ATOM 1270 CB ASN 376 1.605 19.772 61.912 1.00 18.97
ATOM 1271 CG ASN 376 0.537 19.124 62.780 1.00 23.13
ATOM 1272 OD1 ASN 376 -0.527 18.732 62.289 1.00 19.72
ATOM 1273 ND2 ASN 376 0.827 18.989 64.081 1.00 21.10
ATOM 1274 C ASN 376 -0.088 21.080 60.641 1.00 17.80
ATOM 1275 O ASN 376 -0.043 22.028 61.412 1.00 18.77
ATOM 1276 N PRO 377 -1.188 20.820 59.909 1.00 20.03
ATOM 1277 CD PRO 377 -1.463 19.684 59.010 1.00 19.34
ATOM 1278 CA PRO 377 -2.342 21.728 60.011 1.00 20.40
ATOM 1279 CB PRO 377 -3.239 21.293 58.858 1.00 18.78
ATOM 1280 CG PRO 377 -2.979 19.796 58.774 1.00 19.22
ATOM 1281 C PRO 377 -3.086 21.705 61.336 1.00 21.89
ATOM 1282 O PRO 377 -3.922 22.583 61.594 1.00 22.57
ATOM 1283 N ASP 378 -2.771 20.723 62.177 1.00 20.09
ATOM 1284 CA ASP 378 -3.444 20.609 63.463 1.00 22.47
ATOM 1285 CB ASP 378 -3.608 19.131 63.809 1.00 23.71
ATOM 1286 CG ASP 378 -4.555 18.426 62.847 1.00 25.43

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ATOM  1287  OD1 ASP  378     -5.579  19.028  62.487  1.00 28.35
ATOM  1288  OD2 ASP  378     -4.289  17.283  62.443  1.00 30.58
ATOM  1289  C   ASP  378     -2.823  21.403  64.603  1.00 22.30
ATOM  1290  O   ASP  378     -3.265  21.309  65.760  1.00 22.98
ATOM  1291  N   VAL  379     -1.793  22.181  64.279  1.00 22.51
ATOM  1292  CA  VAL  379     -1.167  23.053  65.266  1.00 21.52
ATOM  1293  CB  VAL  379      0.044  23.807  64.662  1.00 20.60
ATOM  1294  CG1 VAL  379      0.424  25.004  65.532  1.00 22.27
ATOM  1295  CG2 VAL  379      1.226  22.848  64.516  1.00 22.31
ATOM  1296  C   VAL  379     -2.255  24.048  65.658  1.00 23.83
ATOM  1297  O   VAL  379     -2.918  24.655  64.793  1.00 25.06
ATOM  1298  N   LYS  380     -2.460  24.212  66.958  1.00 23.33
ATOM  1299  CA  LYS  380     -3.490  25.124  67.430  1.00 24.49
ATOM  1300  CB  LYS  380     -3.797  24.829  68.904  1.00 25.21
ATOM  1301  CG  LYS  380     -4.182  23.365  69.131  1.00 28.03
ATOM  1302  CD  LYS  380     -4.460  23.035  70.594  1.00 30.82
ATOM  1303  CE  LYS  380     -4.728  21.536  70.758  1.00 31.68
ATOM  1304  NZ  LYS  380     -4.904  21.079  72.177  1.00 33.50
ATOM  1305  C   LYS  380     -3.055  26.573  67.250  1.00 24.85
ATOM  1306  O   LYS  380     -1.874  26.891  67.408  1.00 25.55
ATOM  1307  N   GLY  381     -3.988  27.445  66.861  1.00 24.69
ATOM  1308  CA  GLY  381     -3.647  28.852  66.704  1.00 26.29
ATOM  1309  C   GLY  381     -3.384  29.378  65.295  1.00 25.30
ATOM  1310  O   GLY  381     -3.246  30.598  65.093  1.00 27.29
ATOM  1311  N   LEU  382     -3.313  28.490  64.311  1.00 26.35
ATOM  1312  CA  LEU  382     -3.054  28.914  62.941  1.00 26.95
ATOM  1313  CB  LEU  382     -2.997  27.706  61.995  1.00 25.01
ATOM  1314  CG  LEU  382     -1.865  26.700  62.265  1.00 24.87
ATOM  1315  CD1 LEU  382     -2.011  25.507  61.314  1.00 24.53
ATOM  1316  CD2 LEU  382     -0.518  27.384  62.064  1.00 24.40
ATOM  1317  C   LEU  382     -4.120  29.885  62.428  1.00 28.77
ATOM  1318  O   LEU  382     -5.310  29.719  62.695  1.00 28.39
ATOM  1319  N   LYS  383     -3.660  30.881  61.681  1.00 30.83
ATOM  1320  CA  LYS  383     -4.518  31.894  61.078  1.00 32.60
ATOM  1321  CB  LYS  383     -3.670  33.104  60.699  1.00 35.65
ATOM  1322  CG  LYS  383     -4.352  34.121  59.788  1.00 40.31
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ATOM 1323 CD LYS 383 -5.044 35.203 60.589 1.00 42.92
ATOM 1324 CE LYS 383 -5.436 36.376 59.702 1.00 43.80
ATOM 1325 NZ LYS 383 -6.040 37.476 60.505 1.00 44.52
ATOM 1326 C LYS 383 -5.159 31.313 59.819 1.00 32.46
ATOM 1327 O LYS 383 -6.374 31.411 59.620 1.00 33.42
ATOM 1328 N ASN 384 -4.332 30.700 58.977 1.00 30.19
ATOM 1329 CA ASN 384 -4.794 30.118 57.720 1.00 29.86
ATOM 1330 CB ASN 384 -4.154 30.854 56.549 1.00 32.74
ATOM 1331 CG ASN 384 -4.460 32.336 56.570 1.00 36.46
ATOM 1332 OD1 ASN 384 -5.625 32.730 56.585 1.00 39.59
ATOM 1333 ND2 ASN 384 -3.418 33.166 56.583 1.00 37.88
ATOM 1334 C ASN 384 -4.466 28.636 57.636 1.00 26.29
ATOM 1335 O ASN 384 -3.558 28.229 56.912 1.00 26.38
ATOM 1336 N ARG 385 -5.218 27.845 58.387 1.00 24.62
ATOM 1337 CA ARG 385 -5.005 26.406 58.431 1.00 24.85
ATOM 1338 CB ARG 385 -5.994 25.779 59.413 1.00 24.62
ATOM 1339 CG ARG 385 -5.910 24.275 59.561 1.00 27.77
ATOM 1340 CD ARG 385 -6.705 23.839 60.785 1.00 30.37
ATOM 1341 NE ARG 385 -5.976 24.188 62.004 1.00 31.78
ATOM 1342 CZ ARG 385 -6.329 25.148 62.849 1.00 31.80
ATOM 1343 NH1 ARG 385 -7.432 25.867 62.629 1.00 31.71
ATOM 1344 NH2 ARG 385 -5.542 25.426 63.886 1.00 28.60
ATOM 1345 C ARG 385 -5.079 25.727 57.070 1.00 24.38
ATOM 1346 O ARG 385 -4.289 24.824 56.783 1.00 24.23
ATOM 1347 N GLN 386 -6.003 26.165 56.214 1.00 24.39
ATOM 1348 CA GLN 386 -6.128 25.542 54.906 1.00 25.99
ATOM 1349 CB GLN 386 -7.320 26.124 54.128 1.00 29.68
ATOM 1350 CG GLN 386 -7.256 27.619 53.863 1.00 34.93
ATOM 1351 CD GLN 386 -7.246 28.442 55.136 1.00 37.35
ATOM 1352 OE1 GLN 386 -8.016 28.183 56.072 1.00 39.44
ATOM 1353 NE2 GLN 386 -6.373 29.443 55.183 1.00 39.95
ATOM 1354 C GLN 386 -4.867 25.646 54.067 1.00 24.30
ATOM 1355 O GLN 386 -4.561 24.727 53.318 1.00 25.10
ATOM 1356 N GLU 387 -4.140 26.752 54.182 1.00 25.50
ATOM 1357 CA GLU 387 -2.907 26.905 53.413 1.00 25.38
ATOM 1358 CB GLU 387 -2.358 28.328 53.594 1.00 29.21

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ATOM  1359  CG  GLU  387     -3.234  29.420  52.915  1.00 33.12
ATOM  1360  CD  GLU  387     -2.845  30.838  53.284  1.00 37.28
ATOM  1361  OE1 GLU  387     -1.634  31.125  53.407  1.00 40.75
ATOM  1362  OE2 GLU  387     -3.750  31.691  53.436  1.00 38.95
ATOM  1363  C   GLU  387     -1.877  25.841  53.852  1.00 25.54
ATOM  1364  O   GLU  387     -1.097  25.329  53.030  1.00 24.67
ATOM  1365  N   VAL  388     -1.897  25.476  55.132  1.00 24.28
ATOM  1366  CA  VAL  388     -0.960  24.447  55.617  1.00 21.40
ATOM  1367  CB  VAL  388     -0.845  24.439  57.168  1.00 19.68
ATOM  1368  CG1 VAL  388      0.182  23.410  57.597  1.00 22.22
ATOM  1369  CG2 VAL  388     -0.477  25.824  57.691  1.00 20.28
ATOM  1370  C   VAL  388     -1.444  23.076  55.178  1.00 22.10
ATOM  1371  O   VAL  388     -0.666  22.211  54.782  1.00 21.10
ATOM  1372  N   GLU  389     -2.750  22.859  55.243  1.00 22.00
ATOM  1373  CA  GLU  389     -3.284  21.577  54.825  1.00 21.41
ATOM  1374  CB  GLU  389     -4.801  21.538  54.987  1.00 22.76
ATOM  1375  CG  GLU  389     -5.358  20.146  54.988  1.00 31.47
ATOM  1376  CD  GLU  389     -6.793  20.093  55.471  1.00 36.14
ATOM  1377  OE1 GLU  389     -7.160  20.927  56.334  1.00 39.74
ATOM  1378  OE2 GLU  389     -7.540  19.204  55.006  1.00 39.63
ATOM  1379  C   GLU  389     -2.936  21.294  53.382  1.00 19.32
ATOM  1380  O   GLU  389     -2.653  20.155  53.025  1.00 21.32
ATOM  1381  N   VAL  390     -3.001  22.313  52.534  1.00 19.72
ATOM  1382  CA  VAL  390     -2.685  22.148  51.125  1.00 19.82
ATOM  1383  CB  VAL  390     -2.950  23.447  50.316  1.00 19.77
ATOM  1384  CG1 VAL  390     -2.307  23.344  48.919  1.00 22.22
ATOM  1385  CG2 VAL  390     -4.442  23.652  50.169  1.00 23.95
ATOM  1386  C   VAL  390     -1.231  21.744  50.924  1.00 20.27
ATOM  1387  O   VAL  390     -0.924  20.894  50.093  1.00 20.79
ATOM  1388  N   LEU  391     -0.334  22.345  51.699  1.00 21.06
ATOM  1389  CA  LEU  391      1.078  22.004  51.552  1.00 19.84
ATOM  1390  CB  LEU  391      1.951  22.982  52.328  1.00 20.90
ATOM  1391  CG  LEU  391      1.895  24.438  51.836  1.00 21.65
ATOM  1392  CD1 LEU  391      2.846  25.283  52.673  1.00 23.70
ATOM  1393  CD2 LEU  391      2.260  24.515  50.351  1.00 25.56
ATOM  1394  C   LEU  391      1.327  20.583  52.031  1.00 19.59
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ATOM	1395	O	LEU	391	2.090	19.837	51.421	1.00	19.63	
ATOM	1396	N	ARG	392	0.680	20.192	53.130	0.50	19.30	AC1
ATOM	1397	CA	ARG	392	0.862	18.823	53.628	0.50	19.65	AC1
ATOM	1398	CB	ARG	392	0.212	18.620	55.016	0.50	19.22	AC1
ATOM	1399	CG	ARG	392	0.060	17.123	55.382	0.50	18.74	AC1
ATOM	1400	CD	ARG	392	-0.380	16.857	56.840	0.50	19.04	AC1
ATOM	1401	NE	ARG	392	0.710	17.001	57.811	0.50	18.30	AC1
ATOM	1402	CZ	ARG	392	0.739	16.427	59.020	0.50	18.32	AC1
ATOM	1403	NH1	ARG	392	-0.262	15.660	59.432	0.50	18.09	AC1
ATOM	1404	NH2	ARG	392	1.783	16.606	59.826	0.50	13.08	AC1
ATOM	1405	C	ARG	392	0.259	17.833	52.624	0.50	19.79	AC1
ATOM	1406	O	ARG	392	0.768	16.730	52.453	0.50	19.90	AC1
ATOM	1407	N	GLU	393	-0.839	18.220	51.976	1.00	19.51	
ATOM	1408	CA	GLU	393	-1.484	17.355	50.979	1.00	21.32	
ATOM	1409	CB	GLU	393	-2.858	17.922	50.575	1.00	23.83	
ATOM	1410	CG	GLU	393	-3.631	17.066	49.588	1.00	29.44	
ATOM	1411	CD	GLU	393	-4.209	15.767	50.173	1.00	34.23	
ATOM	1412	OE1	GLU	393	-3.940	15.434	51.348	1.00	34.71	
ATOM	1413	OE2	GLU	393	-4.952	15.071	49.433	1.00	37.12	
ATOM	1414	C	GLU	393	-0.556	17.210	49.763	1.00	21.12	
ATOM	1415	O	GLU	393	-0.486	16.147	49.157	1.00	20.35	
ATOM	1416	N	LYS	394	0.143	18.287	49.395	1.00	19.98	
ATOM	1417	CA	LYS	394	1.102	18.186	48.302	1.00	21.24	
ATOM	1418	CB	LYS	394	1.787	19.519	48.048	1.00	22.05	
ATOM	1419	CG	LYS	394	0.903	20.468	47.258	1.00	24.02	
ATOM	1420	CD	LYS	394	1.608	21.778	46.964	1.00	25.62	
ATOM	1421	CE	LYS	394	0.690	22.711	46.199	1.00	28.47	
ATOM	1422	NZ	LYS	394	1.369	24.012	45.959	1.00	30.41	
ATOM	1423	C	LYS	394	2.153	17.137	48.667	1.00	22.08	
ATOM	1424	O	LYS	394	2.555	16.341	47.825	1.00	20.82	
ATOM	1425	N	MET	395	2.590	17.136	49.932	1.00	21.43	
ATOM	1426	CA	MET	395	3.607	16.166	50.369	1.00	21.13	
ATOM	1427	CB	MET	395	4.177	16.520	51.746	1.00	24.05	
ATOM	1428	CG	MET	395	5.100	17.680	51.738	1.00	24.66	
ATOM	1429	SD	MET	395	6.457	17.503	50.571	1.00	27.36	
ATOM	1430	CE	MET	395	6.985	15.797	50.738	1.00	23.91	

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ATOM  1431  C   MET  395     3.121  14.744  50.417  1.00 20.46
ATOM  1432  O   MET  395     3.872  13.832  50.095  1.00 22.42
ATOM  1433  N   PHE  396     1.862  14.542  50.827  1.00 20.87
ATOM  1434  CA  PHE  396     1.285  13.202  50.858  1.00 21.65
ATOM  1435  CB  PHE  396    -0.176  13.203  51.374  1.00 20.90
ATOM  1436  CG  PHE  396    -0.320  13.286  52.875  1.00 22.60
ATOM  1437  CD1 PHE  396     0.733  12.996  53.727  1.00 22.79
ATOM  1438  CD2 PHE  396    -1.544  13.640  53.436  1.00 23.58
ATOM  1439  CE1 PHE  396     0.570  13.063  55.116  1.00 20.29
ATOM  1440  CE2 PHE  396    -1.712  13.702  54.826  1.00 23.72
ATOM  1441  CZ  PHE  396    -0.655  13.416  55.669  1.00 22.24
ATOM  1442  C   PHE  396     1.281  12.652  49.429  1.00 22.43
ATOM  1443  O   PHE  396     1.635  11.494  49.215  1.00 21.80
ATOM  1444  N   LEU  397     0.844  13.462  48.458  1.00 22.96
ATOM  1445  CA  LEU  397     0.813  13.022  47.061  1.00 21.97
ATOM  1446  CB  LEU  397     0.139  14.099  46.176  1.00 22.88
ATOM  1447  CG  LEU  397    -1.385  14.161  46.354  1.00 23.93
ATOM  1448  CD1 LEU  397    -1.981  15.078  45.315  1.00 25.27
ATOM  1449  CD2 LEU  397    -1.972  12.759  46.190  1.00 25.99
ATOM  1450  C   LEU  397     2.233  12.705  46.560  1.00 24.94
ATOM  1451  O   LEU  397     2.450  11.692  45.873  1.00 25.61
ATOM  1452  N   CYS  398     3.195  13.548  46.924  1.00 23.80
ATOM  1453  CA  CYS  398     4.593  13.333  46.519  1.00 26.51
ATOM  1454  CB  CYS  398     5.509  14.454  47.041  1.00 28.87
ATOM  1455  SG  CYS  398     5.551  15.910  46.032  1.00 39.48
ATOM  1456  C   CYS  398     5.111  12.027  47.090  1.00 25.35
ATOM  1457  O   CYS  398     5.738  11.221  46.399  1.00 25.03
ATOM  1458  N   LEU  399     4.861  11.821  48.371  1.00 24.81
ATOM  1459  CA  LEU  399     5.366  10.620  49.009  1.00 24.04
ATOM  1460  CB  LEU  399     5.232  10.739  50.530  1.00 24.26
ATOM  1461  CG  LEU  399     5.806   9.580  51.344  1.00 24.01
ATOM  1462  CD1 LEU  399     7.281   9.343  50.985  1.00 22.08
ATOM  1463  CD2 LEU  399     5.672   9.931  52.821  1.00 22.85
ATOM  1464  C   LEU  399     4.715   9.352  48.518  1.00 26.35
ATOM  1465  O   LEU  399     5.398   8.363  48.267  1.00 25.02
ATOM  1466  N   ASP  400     3.391   9.377  48.361  1.00 27.30
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ATOM	1467	CA	ASP	400	2.680	8.200	47.874	1.00	29.09
ATOM	1468	CB	ASP	400	1.179	8.490	47.772	1.00	31.25
ATOM	1469	CG	ASP	400	0.379	7.258	47.400	1.00	34.75
ATOM	1470	OD1	ASP	400	0.236	6.356	48.252	1.00	35.16
ATOM	1471	OD2	ASP	400	-0.091	7.188	46.250	1.00	38.49
ATOM	1472	C	ASP	400	3.217	7.816	46.497	1.00	28.91
ATOM	1473	O	ASP	400	3.436	6.642	46.212	1.00	29.66
ATOM	1474	N	GLU	401	3.420	8.813	45.644	1.00	28.16
ATOM	1475	CA	GLU	401	3.936	8.577	44.299	1.00	29.87
ATOM	1476	CB	GLU	401	4.052	9.895	43.533	1.00	32.50
ATOM	1477	CG	GLU	401	4.735	9.751	42.180	1.00	38.83
ATOM	1478	CD	GLU	401	4.784	11.048	41.406	1.00	42.93
ATOM	1479	OE1	GLU	401	5.449	12.003	41.865	1.00	45.46
ATOM	1480	OE2	GLU	401	4.147	11.114	40.334	1.00	45.87
ATOM	1481	C	GLU	401	5.308	7.911	44.360	1.00	31.19
ATOM	1482	O	GLU	401	5.574	6.926	43.650	1.00	31.37
ATOM	1483	N	TYR	402	6.171	8.444	45.224	1.00	28.55
ATOM	1484	CA	TYR	402	7.516	7.918	45.365	1.00	29.01
ATOM	1485	CB	TYR	402	8.314	8.737	46.384	1.00	27.40
ATOM	1486	CG	TYR	402	9.667	8.134	46.659	1.00	27.45
ATOM	1487	CD1	TYR	402	9.849	7.238	47.709	1.00	27.18
ATOM	1488	CE1	TYR	402	11.087	6.635	47.933	1.00	28.15
ATOM	1489	CD2	TYR	402	10.747	8.419	45.834	1.00	27.22
ATOM	1490	CE2	TYR	402	11.996	7.820	46.050	1.00	30.03
ATOM	1491	CZ	TYR	402	12.147	6.936	47.097	1.00	30.78
ATOM	1492	OH	TYR	402	13.374	6.358	47.316	1.00	31.66
ATOM	1493	C	TYR	402	7.503	6.453	45.769	1.00	30.16
ATOM	1494	O	TYR	402	8.206	5.641	45.187	1.00	29.67
ATOM	1495	N	CYS	403	6.700	6.113	46.763	1.00	30.42
ATOM	1496	CA	CYS	403	6.616	4.739	47.215	1.00	34.32
ATOM	1497	CB	CYS	403	5.691	4.650	48.430	1.00	33.37
ATOM	1498	SG	CYS	403	6.357	5.485	49.920	1.00	31.63
ATOM	1499	C	CYS	403	6.116	3.820	46.104	1.00	36.81
ATOM	1500	O	CYS	403	6.612	2.703	45.936	1.00	36.95
ATOM	1501	N	ARG	404	5.140	4.289	45.335	1.00	39.50
ATOM	1502	CA	ARG	404	4.597	3.453	44.271	1.00	42.67

ATOM	1503	CB	ARG	404	3.280	4.045	43.746	1.00	43.44
ATOM	1504	CG	ARG	404	2.135	3.802	44.718	1.00	46.08
ATOM	1505	CD	ARG	404	0.746	4.164	44.188	1.00	46.89
ATOM	1506	NE	ARG	404	0.490	5.602	44.159	1.00	46.69
ATOM	1507	CZ	ARG	404	0.733	6.386	43.116	1.00	47.48
ATOM	1508	NH1	ARG	404	1.241	5.874	42.002	1.00	48.94
ATOM	1509	NH2	ARG	404	0.462	7.684	43.181	1.00	48.22
ATOM	1510	C	ARG	404	5.578	3.206	43.137	1.00	43.67
ATOM	1511	O	ARG	404	5.640	2.102	42.598	1.00	44.97
ATOM	1512	N	ARG	405	6.356	4.220	42.785	1.00	45.45
ATOM	1513	CA	ARG	405	7.330	4.098	41.710	1.00	47.72
ATOM	1514	CB	ARG	405	7.700	5.481	41.167	1.00	49.80
ATOM	1515	CG	ARG	405	6.535	6.298	40.624	1.00	53.09
ATOM	1516	CD	ARG	405	7.005	7.695	40.233	1.00	56.62
ATOM	1517	NE	ARG	405	5.931	8.506	39.661	1.00	59.35
ATOM	1518	CZ	ARG	405	5.356	8.263	38.488	1.00	60.20
ATOM	1519	NH1	ARG	405	5.753	7.231	37.756	1.00	61.80
ATOM	1520	NH2	ARG	405	4.382	9.049	38.046	1.00	60.75
ATOM	1521	C	ARG	405	8.609	3.410	42.166	1.00	48.23
ATOM	1522	O	ARG	405	9.078	2.464	41.528	1.00	48.90
ATOM	1523	N	SER	406	9.163	3.891	43.278	1.00	47.66
ATOM	1524	CA	SER	406	10.421	3.382	43.819	1.00	48.66
ATOM	1525	CB	SER	406	11.099	4.477	44.638	1.00	49.49
ATOM	1526	OG	SER	406	11.118	5.698	43.919	1.00	51.64
ATOM	1527	C	SER	406	10.336	2.112	44.656	1.00	48.77
ATOM	1528	O	SER	406	11.355	1.507	44.968	1.00	48.91
ATOM	1529	N	ARG	407	9.129	1.711	45.026	1.00	49.27
ATOM	1530	CA	ARG	407	8.948	0.500	45.813	1.00	50.47
ATOM	1531	CB	ARG	407	9.106	0.811	47.302	1.00	52.25
ATOM	1532	CG	ARG	407	10.476	0.434	47.849	1.00	54.88
ATOM	1533	CD	ARG	407	10.942	1.401	48.918	1.00	55.39
ATOM	1534	NE	ARG	407	12.157	0.927	49.573	1.00	56.11
ATOM	1535	CZ	ARG	407	12.885	1.653	50.416	1.00	56.40
ATOM	1536	NH1	ARG	407	12.524	2.895	50.707	1.00	56.21
ATOM	1537	NH2	ARG	407	13.973	1.133	50.972	1.00	55.90
ATOM	1538	C	ARG	407	7.586	-0.110	45.535	1.00	50.00

ATOM	1539	O	ARG	407	6.847	-0.468	46.451	1.00	50.06
ATOM	1540	N	SER	408	7.279	-0.233	44.248	1.00	49.76
ATOM	1541	CA	SER	408	6.010	-0.777	43.782	1.00	49.98
ATOM	1542	CB	SER	408	6.060	-0.957	42.262	1.00	50.23
ATOM	1543	OG	SER	408	7.129	-1.806	41.880	1.00	50.48
ATOM	1544	C	SER	408	5.622	-2.100	44.439	1.00	49.86
ATOM	1545	O	SER	408	4.444	-2.354	44.698	1.00	50.10
ATOM	1546	N	SER	409	6.620	-2.933	44.706	1.00	50.01
ATOM	1547	CA	SER	409	6.412	-4.245	45.307	1.00	49.71
ATOM	1548	CB	SER	409	7.704	-5.055	45.217	1.00	50.85
ATOM	1549	OG	SER	409	8.799	-4.306	45.730	1.00	52.55
ATOM	1550	C	SER	409	5.954	-4.195	46.758	1.00	49.15
ATOM	1551	O	SER	409	5.476	-5.195	47.300	1.00	48.48
ATOM	1552	N	GLU	410	6.095	-3.035	47.392	1.00	47.66
ATOM	1553	CA	GLU	410	5.701	-2.912	48.785	1.00	45.50
ATOM	1554	CB	GLU	410	6.787	-2.197	49.577	1.00	46.29
ATOM	1555	CG	GLU	410	8.079	-2.980	49.712	1.00	47.76
ATOM	1556	CD	GLU	410	9.074	-2.261	50.592	1.00	48.13
ATOM	1557	OE1	GLU	410	10.155	-1.882	50.092	1.00	49.66
ATOM	1558	OE2	GLU	410	8.761	-2.063	51.784	1.00	48.57
ATOM	1559	C	GLU	410	4.373	-2.197	48.973	1.00	44.10
ATOM	1560	O	GLU	410	4.311	-0.974	49.114	1.00	41.70
ATOM	1561	N	GLU	411	3.306	-2.985	48.986	1.00	42.76
ATOM	1562	CA	GLU	411	1.973	-2.451	49.154	1.00	41.57
ATOM	1563	CB	GLU	411	0.945	-3.529	48.814	1.00	44.42
ATOM	1564	CG	GLU	411	1.166	-4.132	47.439	1.00	48.49
ATOM	1565	CD	GLU	411	0.151	-5.191	47.100	1.00	49.60
ATOM	1566	OE1	GLU	411	0.111	-6.226	47.806	1.00	49.80
ATOM	1567	OE2	GLU	411	-0.605	-4.979	46.129	1.00	50.58
ATOM	1568	C	GLU	411	1.805	-2.000	50.594	1.00	38.78
ATOM	1569	O	GLU	411	2.254	-2.682	51.526	1.00	38.53
ATOM	1570	N	GLY	412	1.170	-0.845	50.768	1.00	34.78
ATOM	1571	CA	GLY	412	0.953	-0.313	52.103	1.00	32.19
ATOM	1572	C	GLY	412	2.163	0.402	52.695	1.00	29.28
ATOM	1573	O	GLY	412	2.133	0.770	53.865	1.00	28.68
ATOM	1574	N	ARG	413	3.207	0.625	51.901	1.00	28.70

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ATOM  1575 CA  ARG  413      4.413   1.286  52.407  1.00 27.65
ATOM  1576 CB  ARG  413      5.513   1.319  51.348  1.00 29.50
ATOM  1577 CG  ARG  413      6.850   1.839  51.905  1.00 29.56
ATOM  1578 CD  ARG  413      8.004   1.721  50.903  1.00 32.68
ATOM  1579 NE  ARG  413      9.242   2.244  51.484  1.00 34.48
ATOM  1580 CZ  ARG  413      9.951   1.632  52.433  1.00 35.49
ATOM  1581 NH1 ARG  413      9.569   0.454  52.914  1.00 34.87
ATOM  1582 NH2 ARG  413     11.036   2.221  52.929  1.00 35.73
ATOM  1583 C   ARG  413      4.153   2.715  52.874  1.00 27.61
ATOM  1584 O   ARG  413      4.656   3.142  53.911  1.00 26.64
ATOM  1585 N   PHE  414      3.377   3.447  52.091  1.00 27.23
ATOM  1586 CA  PHE  414      3.025   4.829  52.406  1.00 25.72
ATOM  1587 CB  PHE  414      2.109   5.368  51.290  1.00 27.69
ATOM  1588 CG  PHE  414      1.553   6.756  51.552  1.00 26.95
ATOM  1589 CD1 PHE  414      2.359   7.882  51.454  1.00 28.43
ATOM  1590 CD2 PHE  414      0.217   6.921  51.891  1.00 29.19
ATOM  1591 CE1 PHE  414      1.842   9.165  51.692  1.00 28.49
ATOM  1592 CE2 PHE  414     -0.315   8.199  52.134  1.00 29.46
ATOM  1593 CZ  PHE  414      0.503   9.325  52.033  1.00 28.75
ATOM  1594 C   PHE  414      2.336   4.891  53.777  1.00 26.40
ATOM  1595 O   PHE  414      2.691   5.702  54.637  1.00 26.65
ATOM  1596 N   ALA  415      1.355   4.027  53.997  1.00 25.07
ATOM  1597 CA  ALA  415      0.652   4.002  55.271  1.00 24.63
ATOM  1598 CB  ALA  415     -0.531   3.028  55.193  1.00 23.72
ATOM  1599 C   ALA  415      1.572   3.622  56.436  1.00 24.02
ATOM  1600 O   ALA  415      1.433   4.142  57.547  1.00 23.15
ATOM  1601 N   ALA  416      2.518   2.722  56.174  1.00 24.35
ATOM  1602 CA  ALA  416      3.448   2.270  57.205  1.00 24.54
ATOM  1603 CB  ALA  416      4.313   1.143  56.666  1.00 24.42
ATOM  1604 C   ALA  416      4.319   3.436  57.639  1.00 23.97
ATOM  1605 O   ALA  416      4.544   3.646  58.832  1.00 25.89
ATOM  1606 N   LEU  417      4.799   4.192  56.664  1.00 23.99
ATOM  1607 CA  LEU  417      5.638   5.348  56.952  1.00 23.65
ATOM  1608 CB  LEU  417      6.056   6.013  55.651  1.00 23.88
ATOM  1609 CG  LEU  417      6.940   5.132  54.768  1.00 22.81
ATOM  1610 CD1 LEU  417      7.104   5.745  53.381  1.00 25.97
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ATOM	1611	CD2	LEU	417	8.313	4.978	55.464	1.00	24.86
ATOM	1612	C	LEU	417	4.894	6.346	57.843	1.00	23.64
ATOM	1613	O	LEU	417	5.434	6.825	58.851	1.00	24.26
ATOM	1614	N	LEU	418	3.635	6.632	57.517	1.00	22.96
ATOM	1615	CA	LEU	418	2.896	7.617	58.305	1.00	22.78
ATOM	1616	CB	LEU	418	1.555	7.961	57.622	1.00	22.19
ATOM	1617	CG	LEU	418	1.632	8.536	56.193	1.00	22.93
ATOM	1618	CD1	LEU	418	0.232	8.983	55.715	1.00	23.88
ATOM	1619	CD2	LEU	418	2.554	9.749	56.179	1.00	23.65
ATOM	1620	C	LEU	418	2.646	7.201	59.762	1.00	24.12
ATOM	1621	O	LEU	418	2.372	8.046	60.620	1.00	22.61
ATOM	1622	N	LEU	419	2.706	5.901	60.049	1.00	25.06
ATOM	1623	CA	LEU	419	2.496	5.440	61.404	1.00	27.92
ATOM	1624	CB	LEU	419	2.406	3.909	61.451	1.00	31.65
ATOM	1625	CG	LEU	419	1.114	3.343	60.884	1.00	34.11
ATOM	1626	CD1	LEU	419	1.026	1.848	61.218	1.00	36.06
ATOM	1627	CD2	LEU	419	-0.068	4.081	61.480	1.00	34.83
ATOM	1628	C	LEU	419	3.594	5.891	62.360	1.00	29.85
ATOM	1629	O	LEU	419	3.400	5.885	63.574	1.00	31.55
ATOM	1630	N	ARG	420	4.736	6.296	61.828	1.00	31.33
ATOM	1631	CA	ARG	420	5.801	6.725	62.718	1.00	31.87
ATOM	1632	CB	ARG	420	7.145	6.755	61.985	1.00	32.74
ATOM	1633	CG	ARG	420	7.648	5.387	61.490	1.00	33.67
ATOM	1634	CD	ARG	420	7.856	4.364	62.622	1.00	36.93
ATOM	1635	NE	ARG	420	6.709	3.481	62.820	1.00	35.35
ATOM	1636	CZ	ARG	420	6.179	3.194	64.003	1.00	37.82
ATOM	1637	NH1	ARG	420	6.692	3.714	65.116	1.00	39.26
ATOM	1638	NH2	ARG	420	5.112	2.408	64.079	1.00	39.04
ATOM	1639	C	ARG	420	5.477	8.092	63.303	1.00	32.15
ATOM	1640	O	ARG	420	5.995	8.456	64.362	1.00	31.60
ATOM	1641	N	LEU	421	4.591	8.845	62.655	1.00	30.38
ATOM	1642	CA	LEU	421	4.278	10.175	63.164	1.00	29.53
ATOM	1643	CB	LEU	421	3.519	10.976	62.121	1.00	30.72
ATOM	1644	CG	LEU	421	4.322	11.027	60.808	1.00	31.31
ATOM	1645	CD1	LEU	421	3.645	12.019	59.885	1.00	32.38
ATOM	1646	CD2	LEU	421	5.800	11.411	61.053	1.00	31.74

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ATOM  1647  C   LEU  421     3.582  10.256  64.521  1.00 28.39
ATOM  1648  O   LEU  421     3.977  11.061  65.363  1.00 26.36
ATOM  1649  N   PRO  422     2.533   9.446  64.762  1.00 27.69
ATOM  1650  CD  PRO  422     1.678   8.672  63.839  1.00 27.47
ATOM  1651  CA  PRO  422     1.915   9.559  66.090  1.00 26.04
ATOM  1652  CB  PRO  422     0.717   8.603  66.005  1.00 28.29
ATOM  1653  CG  PRO  422     0.350   8.664  64.557  1.00 28.91
ATOM  1654  C   PRO  422     2.906   9.143  67.198  1.00 25.36
ATOM  1655  O   PRO  422     2.832   9.637  68.322  1.00 24.06
ATOM  1656  N   ALA  423     3.821   8.228  66.872  1.00 24.34
ATOM  1657  CA  ALA  423     4.817   7.779  67.840  1.00 22.88
ATOM  1658  CB  ALA  423     5.589   6.599  67.273  1.00 26.29
ATOM  1659  C   ALA  423     5.765   8.942  68.158  1.00 24.20
ATOM  1660  O   ALA  423     6.094   9.197  69.315  1.00 22.14
ATOM  1661  N   LEU  424     6.212   9.640  67.119  1.00 22.92
ATOM  1662  CA  LEU  424     7.103  10.773  67.309  1.00 22.78
ATOM  1663  CB  LEU  424     7.512  11.306  65.936  1.00 23.40
ATOM  1664  CG  LEU  424     8.405  12.531  65.875  1.00 24.54
ATOM  1665  CD1 LEU  424     9.777  12.226  66.517  1.00 22.52
ATOM  1666  CD2 LEU  424     8.589  12.892  64.405  1.00 22.78
ATOM  1667  C   LEU  424     6.422  11.861  68.153  1.00 22.46
ATOM  1668  O   LEU  424     7.036  12.468  69.038  1.00 21.68
ATOM  1669  N   ARG  425     5.136  12.101  67.900  1.00 22.38
ATOM  1670  CA  ARG  425     4.386  13.095  68.663  1.00 23.67
ATOM  1671  CB  ARG  425     2.969  13.240  68.087  1.00 26.56
ATOM  1672  CG  ARG  425     2.066  14.140  68.903  1.00 30.90
ATOM  1673  CD  ARG  425     0.977  14.732  68.031  1.00 36.25
ATOM  1674  NE  ARG  425     0.469  13.774  67.044  1.00 40.86
ATOM  1675  CZ  ARG  425    -0.070  12.592  67.339  1.00 42.76
ATOM  1676  NH1 ARG  425    -0.183  12.196  68.604  1.00 46.63
ATOM  1677  NH2 ARG  425    -0.498  11.800  66.367  1.00 44.97
ATOM  1678  C   ARG  425     4.309  12.737  70.150  1.00 21.12
ATOM  1679  O   ARG  425     4.418  13.604  71.021  1.00 21.30
ATOM  1680  N   SER  426     4.124  11.452  70.436  1.00 19.60
ATOM  1681  CA  SER  426     4.021  10.989  71.820  1.00 19.49
ATOM  1682  CB  SER  426     3.534   9.539  71.855  1.00 20.63
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ATOM  1683  OG  SER  426      3.491   9.086  73.198  1.00 23.17
ATOM  1684  C   SER  426      5.374  11.096  72.535  1.00 17.38
ATOM  1685  O   SER  426      5.458  11.496  73.698  1.00 18.97
ATOM  1686  N   ILE  427      6.419  10.742  71.812  1.00 18.11
ATOM  1687  CA  ILE  427      7.770  10.812  72.368  1.00 15.88
ATOM  1688  CB  ILE  427      8.763  10.095  71.449  1.00 15.75
ATOM  1689  CG2 ILE  427     10.213  10.351  71.913  1.00 17.78
ATOM  1690  CG1 ILE  427      8.479   8.591  71.526  1.00 18.23
ATOM  1691  CD1 ILE  427      9.082   7.789  70.440  1.00 20.33
ATOM  1692  C   ILE  427      8.146  12.272  72.599  1.00 16.69
ATOM  1693  O   ILE  427      8.779  12.589  73.606  1.00 16.41
ATOM  1694  N   SER  428      7.767  13.159  71.685  1.00 17.02
ATOM  1695  CA  SER  428      8.059  14.590  71.884  1.00 17.37
ATOM  1696  CB  SER  428      7.636  15.393  70.633  1.00 18.11
ATOM  1697  OG  SER  428      7.745  16.794  70.876  1.00 19.14
ATOM  1698  C   SER  428      7.377  15.138  73.154  1.00 18.08
ATOM  1699  O   SER  428      7.968  15.916  73.928  1.00 16.98
ATOM  1700  N   LEU  429      6.134  14.741  73.425  1.00 18.84
ATOM  1701  CA  LEU  429      5.518  15.249  74.633  1.00 19.23
ATOM  1702  CB  LEU  429      4.054  14.807  74.723  1.00 22.17
ATOM  1703  CG  LEU  429      3.187  15.432  73.625  1.00 25.96
ATOM  1704  CD1 LEU  429      1.800  14.809  73.624  1.00 28.92
ATOM  1705  CD2 LEU  429      3.087  16.943  73.855  1.00 29.57
ATOM  1706  C   LEU  429      6.296  14.782  75.860  1.00 17.99
ATOM  1707  O   LEU  429      6.465  15.527  76.816  1.00 18.52
ATOM  1708  N   LYS  430      6.778  13.544  75.830  1.00 18.39
ATOM  1709  CA  LYS  430      7.540  13.047  76.957  1.00 17.66
ATOM  1710  CB  LYS  430      7.780  11.544  76.826  1.00 19.73
ATOM  1711  CG  LYS  430      8.539  10.975  78.020  1.00 23.74
ATOM  1712  CD  LYS  430      7.625  11.004  79.260  1.00 27.95
ATOM  1713  CE  LYS  430      8.192  10.194  80.414  1.00 34.36
ATOM  1714  NZ  LYS  430      7.167  10.122  81.490  1.00 36.64
ATOM  1715  C   LYS  430      8.865  13.795  77.077  1.00 18.37
ATOM  1716  O   LYS  430      9.346  14.034  78.191  1.00 18.47
ATOM  1717  N   SER  431      9.435  14.174  75.936  0.50 17.09    AC1
ATOM  1718  CA  SER  431     10.693  14.931  75.919  0.50 18.08    AC1
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ATOM	1719	CB	SER	431	11.102	15.238	74.471	0.50	17.50	AC1
ATOM	1720	OG	SER	431	12.180	16.159	74.413	0.50	19.63	AC1
ATOM	1721	C	SER	431	10.472	16.244	76.663	0.50	18.02	AC1
ATOM	1722	O	SER	431	11.297	16.668	77.464	0.50	17.75	AC1
ATOM	1723	N	PHE	432	9.326	16.875	76.415	1.00	17.68	
ATOM	1724	CA	PHE	432	9.020	18.162	77.057	1.00	17.81	
ATOM	1725	CB	PHE	432	7.778	18.817	76.425	1.00	18.74	
ATOM	1726	CG	PHE	432	8.099	19.713	75.249	1.00	17.54	
ATOM	1727	CD1	PHE	432	8.649	20.976	75.448	1.00	18.72	
ATOM	1728	CD2	PHE	432	7.851	19.290	73.958	1.00	17.78	
ATOM	1729	CE1	PHE	432	8.941	21.800	74.351	1.00	18.20	
ATOM	1730	CE2	PHE	432	8.135	20.093	72.863	1.00	18.04	
ATOM	1731	CZ	PHE	432	8.684	21.358	73.060	1.00	19.15	
ATOM	1732	C	PHE	432	8.817	17.989	78.550	1.00	18.32	
ATOM	1733	O	PHE	432	9.170	18.872	79.330	1.00	20.66	
ATOM	1734	N	GLU	433	8.249	16.852	78.964	1.00	17.15	
ATOM	1735	CA	GLU	433	8.073	16.592	80.382	1.00	20.50	
ATOM	1736	CB	GLU	433	7.520	15.192	80.613	1.00	19.84	
ATOM	1737	CG	GLU	433	6.045	15.053	80.320	1.00	27.71	
ATOM	1738	CD	GLU	433	5.533	13.688	80.744	1.00	31.07	
ATOM	1739	OE1	GLU	433	5.964	13.224	81.823	1.00	34.98	
ATOM	1740	OE2	GLU	433	4.714	13.094	80.006	1.00	34.76	
ATOM	1741	C	GLU	433	9.437	16.691	81.052	1.00	19.32	
ATOM	1742	O	GLU	433	9.574	17.322	82.106	1.00	20.27	
ATOM	1743	N	HIS	434	10.438	16.059	80.435	1.00	18.45	
ATOM	1744	CA	HIS	434	11.810	16.086	80.972	1.00	19.10	
ATOM	1745	CB	HIS	434	12.708	15.091	80.247	1.00	20.67	
ATOM	1746	CG	HIS	434	12.346	13.662	80.495	1.00	21.88	
ATOM	1747	CD2	HIS	434	12.196	12.621	79.642	1.00	22.64	
ATOM	1748	ND1	HIS	434	12.153	13.151	81.763	1.00	24.64	
ATOM	1749	CE1	HIS	434	11.901	11.857	81.678	1.00	26.38	
ATOM	1750	NE2	HIS	434	11.924	11.509	80.403	1.00	25.49	
ATOM	1751	C	HIS	434	12.448	17.471	80.900	1.00	19.47	
ATOM	1752	O	HIS	434	13.029	17.930	81.868	1.00	20.51	
ATOM	1753	N	LEU	435	12.360	18.122	79.749	1.00	17.30	
ATOM	1754	CA	LEU	435	12.926	19.464	79.614	1.00	17.70	

ATOM	1755	CB	LEU	435	12.660	20.017	78.219	1.00	17.54
ATOM	1756	CG	LEU	435	13.350	19.239	77.100	1.00	17.06
ATOM	1757	CD1	LEU	435	12.933	19.793	75.764	1.00	19.34
ATOM	1758	CD2	LEU	435	14.874	19.343	77.242	1.00	19.09
ATOM	1759	C	LEU	435	12.334	20.411	80.653	1.00	17.96
ATOM	1760	O	LEU	435	13.034	21.260	81.193	1.00	18.73
ATOM	1761	N	PHE	436	11.035	20.302	80.921	1.00	17.35
ATOM	1762	CA	PHE	436	10.460	21.192	81.936	1.00	18.85
ATOM	1763	CB	PHE	436	8.920	21.188	81.897	1.00	19.91
ATOM	1764	CG	PHE	436	8.340	21.916	80.720	1.00	22.43
ATOM	1765	CD1	PHE	436	8.885	23.113	80.288	1.00	23.77
ATOM	1766	CD2	PHE	436	7.243	21.399	80.040	1.00	23.20
ATOM	1767	CE1	PHE	436	8.353	23.783	79.202	1.00	25.60
ATOM	1768	CE2	PHE	436	6.703	22.063	78.942	1.00	22.41
ATOM	1769	CZ	PHE	436	7.250	23.249	78.521	1.00	26.06
ATOM	1770	C	PHE	436	10.916	20.802	83.332	1.00	20.10
ATOM	1771	O	PHE	436	11.195	21.670	84.161	1.00	22.89
ATOM	1772	N	PHE	437	11.001	19.500	83.605	1.00	19.98
ATOM	1773	CA	PHE	437	11.412	19.023	84.922	1.00	21.11
ATOM	1774	CB	PHE	437	11.364	17.484	84.974	1.00	21.57
ATOM	1775	CG	PHE	437	11.628	16.913	86.339	1.00	25.91
ATOM	1776	CD1	PHE	437	10.633	16.924	87.313	1.00	27.17
ATOM	1777	CD2	PHE	437	12.881	16.419	86.665	1.00	27.22
ATOM	1778	CE1	PHE	437	10.891	16.447	88.599	1.00	30.66
ATOM	1779	CE2	PHE	437	13.153	15.942	87.944	1.00	31.40
ATOM	1780	CZ	PHE	437	12.158	15.957	88.910	1.00	29.78
ATOM	1781	C	PHE	437	12.807	19.496	85.305	1.00	22.67
ATOM	1782	O	PHE	437	13.046	19.895	86.464	1.00	24.17
ATOM	1783	N	PHE	438	13.724	19.453	84.346	1.00	19.58
ATOM	1784	CA	PHE	438	15.103	19.888	84.567	1.00	22.15
ATOM	1785	CB	PHE	438	16.038	19.027	83.718	1.00	22.90
ATOM	1786	CG	PHE	438	16.093	17.595	84.171	1.00	23.82
ATOM	1787	CD1	PHE	438	16.725	17.262	85.361	1.00	24.00
ATOM	1788	CD2	PHE	438	15.509	16.584	83.419	1.00	27.39
ATOM	1789	CE1	PHE	438	16.773	15.942	85.795	1.00	25.11
ATOM	1790	CE2	PHE	438	15.557	15.253	83.847	1.00	27.37

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ATOM  1791  CZ  PHE  438     16.188  14.935  85.033  1.00 27.90
ATOM  1792  C   PHE  438     15.334  21.383  84.256  1.00 21.04
ATOM  1793  O   PHE  438     16.454  21.875  84.352  1.00 22.98
ATOM  1794  N   HIS  439     14.267  22.077  83.867  1.00 19.84
ATOM  1795  CA  HIS  439     14.311  23.503  83.508  1.00 19.79
ATOM  1796  CB  HIS  439     14.550  24.380  84.742  1.00 21.68
ATOM  1797  CG  HIS  439     13.463  24.294  85.763  1.00 24.96
ATOM  1798  CD2 HIS  439     12.345  25.037  85.939  1.00 27.66
ATOM  1799  ND1 HIS  439     13.440  23.331  86.747  1.00 26.44
ATOM  1800  CE1 HIS  439     12.353  23.481  87.481  1.00 27.37
ATOM  1801  NE2 HIS  439     11.672  24.511  87.012  1.00 28.08
ATOM  1802  C   HIS  439     15.375  23.803  82.469  1.00 20.93
ATOM  1803  O   HIS  439     16.185  24.726  82.626  1.00 23.42
ATOM  1804  N   LEU  440     15.318  23.068  81.366  1.00 16.51
ATOM  1805  CA  LEU  440     16.289  23.200  80.301  1.00 18.97
ATOM  1806  CB  LEU  440     16.820  21.813  79.917  1.00 19.31
ATOM  1807  CG  LEU  440     17.585  21.101  81.017  1.00 21.82
ATOM  1808  CD1 LEU  440     17.920  19.672  80.567  1.00 24.43
ATOM  1809  CD2 LEU  440     18.839  21.874  81.341  1.00 21.97
ATOM  1810  C   LEU  440     15.751  23.859  79.042  1.00 20.05
ATOM  1811  O   LEU  440     16.497  24.030  78.099  1.00 21.82
ATOM  1812  N   VAL  441     14.478  24.229  79.038  1.00 19.87
ATOM  1813  CA  VAL  441     13.879  24.814  77.833  1.00 21.84
ATOM  1814  CB  VAL  441     12.795  23.830  77.247  1.00 22.63
ATOM  1815  CG1 VAL  441     11.601  23.713  78.192  1.00 22.79
ATOM  1816  CG2 VAL  441     12.365  24.276  75.855  1.00 24.87
ATOM  1817  C   VAL  441     13.306  26.224  78.045  1.00 22.01
ATOM  1818  O   VAL  441     12.587  26.478  79.009  1.00 20.37
ATOM  1819  N   ALA  442     13.646  27.122  77.120  1.00 23.96
ATOM  1820  CA  ALA  442     13.233  28.529  77.172  1.00 27.08
ATOM  1821  CB  ALA  442     14.246  29.393  76.392  1.00 28.21
ATOM  1822  C   ALA  442     11.846  28.718  76.591  1.00 28.96
ATOM  1823  O   ALA  442     11.655  29.494  75.658  1.00 30.12
ATOM  1824  N   ASP  443     10.895  28.011  77.178  1.00 30.46
ATOM  1825  CA  ASP  443      9.493  27.994  76.764  1.00 31.83
ATOM  1826  CB  ASP  443      8.678  27.367  77.906  1.00 33.17
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ATOM	1827	CG	ASP	443	7.208	27.218	77.581	1.00	34.98
ATOM	1828	OD1	ASP	443	6.856	26.945	76.404	1.00	37.47
ATOM	1829	OD2	ASP	443	6.404	27.346	78.524	1.00	31.58
ATOM	1830	C	ASP	443	8.873	29.320	76.318	1.00	31.97
ATOM	1831	O	ASP	443	8.426	29.453	75.180	1.00	30.41
ATOM	1832	N	THR	444	8.854	30.304	77.205	1.00	32.53
ATOM	1833	CA	THR	444	8.236	31.586	76.891	1.00	32.98
ATOM	1834	CB	THR	444	7.965	32.371	78.198	1.00	34.53
ATOM	1835	OG1	THR	444	9.196	32.581	78.900	1.00	37.04
ATOM	1836	CG2	THR	444	7.020	31.577	79.102	1.00	35.95
ATOM	1837	C	THR	444	8.981	32.486	75.901	1.00	32.99
ATOM	1838	O	THR	444	8.399	33.436	75.370	1.00	32.71
ATOM	1839	N	SER	445	10.248	32.179	75.639	1.00	30.56
ATOM	1840	CA	SER	445	11.071	32.977	74.727	1.00	29.90
ATOM	1841	CB	SER	445	12.481	33.132	75.313	1.00	29.52
ATOM	1842	OG	SER	445	12.418	33.766	76.576	1.00	31.76
ATOM	1843	C	SER	445	11.199	32.429	73.308	1.00	29.39
ATOM	1844	O	SER	445	11.580	33.153	72.387	1.00	28.30
ATOM	1845	N	ILE	446	10.875	31.151	73.133	1.00	26.98
ATOM	1846	CA	ILE	446	11.010	30.511	71.840	1.00	25.95
ATOM	1847	CB	ILE	446	10.656	29.013	71.961	1.00	26.36
ATOM	1848	CG2	ILE	446	10.295	28.431	70.595	1.00	24.39
ATOM	1849	CG1	ILE	446	11.864	28.300	72.575	1.00	27.57
ATOM	1850	CD1	ILE	446	11.637	26.869	72.971	1.00	27.13
ATOM	1851	C	ILE	446	10.312	31.144	70.640	1.00	25.28
ATOM	1852	O	ILE	446	10.917	31.247	69.571	1.00	23.47
ATOM	1853	N	ALA	447	9.058	31.549	70.809	1.00	26.37
ATOM	1854	CA	ALA	447	8.316	32.183	69.725	1.00	28.80
ATOM	1855	CB	ALA	447	6.932	32.606	70.219	1.00	30.52
ATOM	1856	C	ALA	447	9.114	33.394	69.218	1.00	28.51
ATOM	1857	O	ALA	447	9.229	33.608	68.005	1.00	29.41
ATOM	1858	N	GLY	448	9.675	34.164	70.155	1.00	28.53
ATOM	1859	CA	GLY	448	10.474	35.337	69.811	1.00	27.89
ATOM	1860	C	GLY	448	11.762	34.993	69.095	1.00	28.77
ATOM	1861	O	GLY	448	12.167	35.692	68.162	1.00	28.23
ATOM	1862	N	TYR	449	12.435	33.927	69.536	1.00	27.26

ATOM	1863	CA	TYR	449	13.666	33.502	68.872	1.00	28.14
ATOM	1864	CB	TYR	449	14.262	32.267	69.553	1.00	26.16
ATOM	1865	CG	TYR	449	14.683	32.492	70.990	1.00	28.82
ATOM	1866	CD1	TYR	449	14.913	33.782	71.482	1.00	29.84
ATOM	1867	CE1	TYR	449	15.336	33.988	72.802	1.00	32.66
ATOM	1868	CD2	TYR	449	14.881	31.412	71.853	1.00	29.90
ATOM	1869	CE2	TYR	449	15.306	31.604	73.173	1.00	30.71
ATOM	1870	CZ	TYR	449	15.532	32.887	73.641	1.00	32.74
ATOM	1871	OH	TYR	449	15.979	33.070	74.939	1.00	36.98
ATOM	1872	C	TYR	449	13.361	33.150	67.420	1.00	27.51
ATOM	1873	O	TYR	449	14.116	33.491	66.513	1.00	27.99
ATOM	1874	N	ILE	450	12.254	32.442	67.207	1.00	27.41
ATOM	1875	CA	ILE	450	11.876	32.053	65.861	1.00	27.70
ATOM	1876	CB	ILE	450	10.662	31.102	65.863	1.00	26.64
ATOM	1877	CG2	ILE	450	10.292	30.744	64.413	1.00	26.88
ATOM	1878	CG1	ILE	450	11.003	29.846	66.690	1.00	27.46
ATOM	1879	CD1	ILE	450	9.811	28.956	67.032	1.00	24.45
ATOM	1880	C	ILE	450	11.534	33.295	65.041	1.00	29.34
ATOM	1881	O	ILE	450	11.994	33.440	63.911	1.00	30.32
ATOM	1882	N	ARG	451	10.735	34.187	65.617	1.00	30.43
ATOM	1883	CA	ARG	451	10.351	35.416	64.923	1.00	33.00
ATOM	1884	CB	ARG	451	9.514	36.306	65.851	1.00	32.56
ATOM	1885	CG	ARG	451	8.874	37.519	65.161	1.00	34.91
ATOM	1886	CD	ARG	451	7.955	38.328	66.076	1.00	36.14
ATOM	1887	NE	ARG	451	6.768	37.599	66.518	1.00	37.46
ATOM	1888	CZ	ARG	451	6.669	36.943	67.672	1.00	40.02
ATOM	1889	NH1	ARG	451	7.690	36.921	68.521	1.00	41.16
ATOM	1890	NH2	ARG	451	5.547	36.299	67.976	1.00	40.59
ATOM	1891	C	ARG	451	11.629	36.138	64.472	1.00	34.57
ATOM	1892	O	ARG	451	11.761	36.516	63.298	1.00	34.59
ATOM	1893	N	ASP	452	12.578	36.304	65.392	1.00	36.05
ATOM	1894	CA	ASP	452	13.837	36.975	65.070	1.00	39.88
ATOM	1895	CB	ASP	452	14.690	37.184	66.331	1.00	42.41
ATOM	1896	CG	ASP	452	14.004	38.065	67.364	1.00	46.01
ATOM	1897	OD1	ASP	452	13.162	38.897	66.961	1.00	46.57
ATOM	1898	OD2	ASP	452	14.315	37.934	68.576	1.00	48.55

ATOM	1899	C	ASP	452	14.657	36.212	64.039	1.00	40.80
ATOM	1900	O	ASP	452	15.219	36.805	63.112	1.00	42.52
ATOM	1901	N	ALA	453	14.730	34.896	64.197	1.00	41.16
ATOM	1902	CA	ALA	453	15.493	34.071	63.272	1.00	42.41
ATOM	1903	CB	ALA	453	15.585	32.643	63.796	1.00	41.71
ATOM	1904	C	ALA	453	14.904	34.070	61.863	1.00	44.06
ATOM	1905	O	ALA	453	15.635	33.910	60.887	1.00	44.96
ATOM	1906	N	LEU	454	13.590	34.259	61.759	1.00	45.34
ATOM	1907	CA	LEU	454	12.921	34.261	60.460	1.00	47.12
ATOM	1908	CB	LEU	454	11.419	33.989	60.631	1.00	42.61
ATOM	1909	CG	LEU	454	11.078	32.514	60.884	1.00	38.89
ATOM	1910	CD1	LEU	454	9.576	32.329	60.950	1.00	36.29
ATOM	1911	CD2	LEU	454	11.660	31.657	59.764	1.00	36.23
ATOM	1912	C	LEU	454	13.149	35.544	59.669	1.00	50.37
ATOM	1913	O	LEU	454	13.255	35.506	58.443	1.00	51.61
ATOM	1914	N	ARG	455	13.218	36.679	60.360	1.00	54.48
ATOM	1915	CA	ARG	455	13.486	37.951	59.688	1.00	58.31
ATOM	1916	CB	ARG	455	13.128	39.147	60.582	1.00	59.22
ATOM	1917	CG	ARG	455	11.635	39.352	60.806	1.00	60.97
ATOM	1918	CD	ARG	455	11.318	40.787	61.228	1.00	62.50
ATOM	1919	NE	ARG	455	10.998	40.919	62.648	1.00	64.04
ATOM	1920	CZ	ARG	455	11.873	40.784	63.640	1.00	64.71
ATOM	1921	NH1	ARG	455	13.146	40.511	63.378	1.00	64.92
ATOM	1922	NH2	ARG	455	11.470	40.923	64.897	1.00	64.48
ATOM	1923	C	ARG	455	14.988	37.938	59.452	1.00	60.72
ATOM	1924	O	ARG	455	15.597	38.964	59.147	1.00	61.55
ATOM	1925	N	ASN	456	15.557	36.743	59.597	1.00	63.01
ATOM	1926	CA	ASN	456	16.983	36.482	59.463	1.00	64.82
ATOM	1927	CB	ASN	456	17.434	36.512	57.987	1.00	66.21
ATOM	1928	CG	ASN	456	17.254	37.871	57.327	1.00	67.51
ATOM	1929	OD1	ASN	456	17.901	38.850	57.702	1.00	68.69
ATOM	1930	ND2	ASN	456	16.377	37.930	56.326	1.00	68.01
ATOM	1931	C	ASN	456	17.795	37.442	60.317	1.00	65.37
ATOM	1932	O	ASN	456	17.456	37.680	61.480	1.00	65.63
ATOM	1933	N	GLY	457	18.858	37.997	59.749	1.00	65.99
ATOM	1934	CA	GLY	457	19.704	38.896	60.510	1.00	66.46

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ATOM  1935  C   GLY   457     20.739  38.015  61.176  1.00 66.78
ATOM  1936  O   GLY   457     21.568  38.471  61.968  1.00 67.21
ATOM  1937  N   GLY   458     20.669  36.728  60.844  1.00 66.86
ATOM  1938  CA  GLY   458     21.594  35.753  61.384  1.00 66.84
ATOM  1939  C   GLY   458     22.018  34.761  60.315  1.00 66.86
ATOM  1940  O   GLY   458     21.450  34.801  59.199  1.00 66.65
ATOM  1941  OXT GLY   458     22.922  33.943  60.593  1.00 65.49
ATOM  1942  OH2 TIP  1003     30.252  23.128  74.386  1.00 27.69
ATOM  1943  OH2 TIP  1005     14.203  25.558  89.644  1.00 25.22
ATOM  1944  OH2 TIP  1006      8.388  25.042  72.262  1.00 22.81
ATOM  1945  OH2 TIP  1008      8.367  21.538  69.460  1.00 19.23
ATOM  1946  OH2 TIP  1009     -7.350  22.030  52.884  1.00 80.11
ATOM  1947  OH2 TIP  1010     -4.017  19.644  67.897  1.00 33.26
ATOM  1948  OH2 TIP  1011      8.365   3.022  77.974  1.00 47.93
ATOM  1949  OH2 TIP  1012     30.690   8.779  67.839  1.00 26.30
ATOM  1950  OH2 TIP  1013     12.264   8.843  80.249  1.00 26.01
ATOM  1951  OH2 TIP  1014     -1.764  16.382  62.652  1.00 44.82
ATOM  1952  OH2 TIP  1015     20.301  34.946  75.498  1.00 51.92
ATOM  1953  OH2 TIP  1016     14.443  15.693  61.296  1.00 22.04
ATOM  1954  OH2 TIP  1017     12.487  31.635  78.951  1.00 36.76
ATOM  1955  OH2 TIP  1018     16.579   6.557  83.739  1.00 27.86
ATOM  1956  OH2 TIP  1019     -0.626  26.615  50.499  1.00 30.82
ATOM  1957  OH2 TIP  1021      3.543  20.127  64.859  1.00 23.80
ATOM  1958  OH2 TIP  1022      4.772   0.996  47.855  1.00 40.67
ATOM  1959  OH2 TIP  1023      9.799  29.451  51.621  1.00 30.93
ATOM  1960  OH2 TIP  1024      7.476  19.030  68.589  1.00 22.30
ATOM  1961  OH2 TIP  1025     20.355   7.131  58.551  1.00 52.44
ATOM  1962  OH2 TIP  1026     -0.829  29.526  57.153  1.00 31.90
ATOM  1963  OH2 TIP  1027     11.560  -6.342  53.442  1.00 52.29
ATOM  1964  OH2 TIP  1028     15.278   0.625  72.808  1.00 27.12
ATOM  1965  OH2 TIP  1029     22.593  26.832  76.012  1.00 35.56
ATOM  1966  OH2 TIP  1031      3.001  25.878  68.078  1.00 22.76
ATOM  1967  OH2 TIP  1032     13.489  25.800  47.958  1.00 47.50
ATOM  1968  OH2 TIP  1033     -7.554  18.088  60.905  1.00 30.53
ATOM  1969  OH2 TIP  1034     24.742  18.595  64.446  1.00 44.88
ATOM  1970  OH2 TIP  1035     13.751  37.059  78.800  1.00 60.77
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ATOM  1971 OH2 TIP  1036     -0.515  10.167  75.163  1.00 36.51
ATOM  1972 OH2 TIP  1037     12.373  35.911  72.901  1.00 32.65
ATOM  1973 OH2 TIP  1039     23.543  26.270  78.523  1.00 24.40
ATOM  1974 OH2 TIP  1040     17.896  20.961  59.259  1.00 39.57
ATOM  1975 OH2 TIP  1041      8.248  15.187  89.930  1.00 59.85
ATOM  1976 OH2 TIP  1042      7.418  31.128  73.133  1.00 34.33
ATOM  1977 OH2 TIP  1043     21.123   8.890  53.894  1.00 67.39
ATOM  1978 OH2 TIP  1045     15.162  18.243  53.355  1.00 28.26
ATOM  1979 OH2 TIP  1050      4.216  23.224  44.827  1.00 46.56
ATOM  1980 OH2 TIP  1051     17.523   1.262  73.909  1.00 23.12
ATOM  1981 OH2 TIP  1052     -0.169  20.149  67.166  1.00 67.45
ATOM  1982 OH2 TIP  1053     20.135  12.837  55.866  1.00 51.70
ATOM  1983 OH2 TIP  1054     10.612  35.387  77.215  1.00 57.20
ATOM  1984 OH2 TIP  1055     14.587  38.805  73.912  1.00 56.14
ATOM  1985 OH2 TIP  1056     22.658  15.094  55.769  1.00 63.46
ATOM  1986 OH2 TIP  1057      8.196   1.415  39.058  1.00 55.65
ATOM  1987 OH2 TIP  1058     10.807   2.725  77.173  1.00 22.15
ATOM  1988 OH2 TIP  1059     19.013  20.604  62.130  1.00 32.43
ATOM  1989 OH2 TIP  1061      2.388  16.861  45.084  1.00 25.70
ATOM  1990 OH2 TIP  1063      5.229   6.816  86.424  1.00 59.99
ATOM  1991 OH2 TIP  1501     18.919  15.965  66.146  1.00 24.36
ATOM  1992 OH2 TIP  1502      2.744  33.258  66.246  1.00 30.10
ATOM  1993 OH2 TIP  1503      4.527  17.244  77.877  1.00 23.98
ATOM  1994 OH2 TIP  1504     -0.815  22.723  68.903  1.00 24.06
ATOM  1995 OH2 TIP  1506     22.697   1.204  69.760  1.00 28.71
ATOM  1996 OH2 TIP  1507     12.438  25.185  81.547  1.00 28.20
ATOM  1997 OH2 TIP  1508     17.107  31.275  76.636  1.00 33.34
ATOM  1998 OH2 TIP  1509     17.900  15.686  59.270  1.00 37.88
ATOM  1999 OH2 TIP  1510      7.197  12.183  44.002  1.00 29.62
ATOM  2000 OH2 TIP  1511     -4.834  15.832  60.463  1.00 33.76
ATOM  2001 OH2 TIP  1512     11.093   1.186  74.736  1.00 29.08
ATOM  2002 OH2 TIP  1513     -0.145   2.568  51.845  1.00 30.78
ATOM  2003 OH2 TIP  1514     -6.100  23.488  73.541  1.00 27.96
ATOM  2004 OH2 TIP  1515      8.298  14.512  44.198  1.00 34.89
ATOM  2005 OH2 TIP  1516      0.418  26.098  68.989  1.00 28.71
ATOM  2006 OH2 TIP  1517     -7.177  16.116  59.030  1.00 32.04
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ATOM 2007 OH2 TIP 1519 18.000 18.387 62.314 1.00 32.49
ATOM 2008 OH2 TIP 1520 21.777 20.403 61.898 1.00 38.66
ATOM 2009 OH2 TIP 1521 -1.379 32.714 63.883 1.00 40.86
ATOM 2010 OH2 TIP 1522 1.931 22.610 68.721 1.00 31.49
ATOM 2011 OH2 TIP 1523 -3.158 9.157 64.790 1.00 46.08
ATOM 2012 OH2 TIP 1524 2.081 4.709 65.432 1.00 38.87
ATOM 2013 OH2 TIP 1525 3.829 11.325 75.940 1.00 34.36
ATOM 2014 OH2 TIP 1527 21.845 33.747 71.839 1.00 51.86
ATOM 2015 OH2 TIP 1528 12.196 0.941 78.760 1.00 46.53
ATOM 2016 OH2 TIP 1529 30.316 21.478 85.009 1.00 28.49
ATOM 2017 OH2 TIP 1530 9.786 2.798 91.182 1.00 58.36
ATOM 2018 OH2 TIP 1531 16.571 8.007 48.772 1.00 38.32
ATOM 2019 OH2 TIP 1532 3.764 24.595 70.409 1.00 31.40
ATOM 2020 OH2 TIP 1533 -0.952 5.111 57.996 1.00 39.42
ATOM 2021 OH2 TIP 1534 8.395 29.793 48.733 1.00 45.92
ATOM 2022 OH2 TIP 1535 18.190 -0.943 54.382 1.00 55.57
ATOM 2023 OH2 TIP 1536 4.583 13.859 64.203 1.00 30.44
ATOM 2024 OH2 TIP 1538 12.012 14.232 84.365 1.00 33.97
ATOM 2025 OH2 TIP 1539 -1.284 36.017 69.736 1.00 57.91
ATOM 2026 OH2 TIP 1540 2.454 15.898 79.022 1.00 40.22
ATOM 2027 OH2 TIP 1544 2.719 2.670 49.088 1.00 32.00
ATOM 2028 OH2 TIP 1545 13.537 37.410 71.136 1.00 41.29
ATOM 2029 OH2 TIP 1546 22.697 0.071 79.248 1.00 32.01
ATOM 2030 OH2 TIP 1548 -0.239 7.542 39.851 1.00 52.37
ATOM 2031 OH2 TIP 1549 0.076 10.603 44.453 1.00 41.67
ATOM 2032 OH2 TIP 1550 31.157 3.039 59.611 1.00 43.66
ATOM 2033 OH2 TIP 1551 4.226 34.045 72.549 1.00 53.58
ATOM 2034 OH2 TIP 1554 10.022 33.359 56.088 1.00 41.48
ATOM 2035 OH2 TIP 1555 -1.058 37.708 61.917 1.00 54.81
ATOM 2036 OH2 TIP 1556 -4.583 15.870 53.480 1.00 37.02
ATOM 2037 OH2 TIP 1557 23.851 8.517 92.595 1.00 36.91
ATOM 2038 OH2 TIP 1558 -7.204 28.744 59.955 1.00 35.72
ATOM 2039 OH2 TIP 1560 19.483 16.334 88.331 1.00 34.61
ATOM 2040 OH2 TIP 1561 1.968 8.086 38.648 1.00 57.90
ATOM 2041 OH2 TIP 1562 32.430 -4.459 71.625 1.00 63.22
ATOM 2042 OH2 TIP 1563 7.819 12.682 83.368 1.00 47.71

ATOM	2043	OH2	TIP	1564	-5.435	18.376	72.810	1.00	41.90
ATOM	2044	OH2	TIP	1565	19.550	17.394	63.917	1.00	31.79
ATOM	2045	OH2	TIP	1566	24.069	28.502	85.703	1.00	50.24
ATOM	2046	OH2	TIP	1568	26.854	12.830	56.392	1.00	51.68
ATOM	2047	OH2	TIP	1570	3.595	32.325	68.760	1.00	45.07
ATOM	2048	OH2	TIP	1571	24.805	8.300	62.036	1.00	28.27
ATOM	2049	OH2	TIP	1572	4.194	17.554	63.640	1.00	26.21
ATOM	2050	OH2	TIP	1573	2.589	20.195	67.352	1.00	34.52
ATOM	2051	OH2	TIP	1574	15.713	17.937	61.017	1.00	52.03
ATOM	2052	OH2	TIP	1575	-9.321	14.210	59.772	1.00	33.92
ATOM	2053	OH2	TIP	1576	13.215	7.332	82.542	1.00	31.45
ATOM	2054	OH2	TIP	1577	10.470	24.539	83.194	1.00	35.29
ATOM	2055	OH2	TIP	1578	25.712	17.999	53.496	1.00	41.46
ATOM	2056	OH2	TIP	1579	9.445	-0.239	41.882	1.00	41.51
ATOM	2057	OH2	TIP	1580	6.603	16.005	42.611	1.00	32.35
ATOM	2058	OH2	TIP	1581	-1.523	7.654	59.739	1.00	50.11
ATOM	2059	OH2	TIP	1582	8.397	34.515	72.891	1.00	33.81
ATOM	2060	OH2	TIP	1583	2.742	39.191	60.949	1.00	39.77
ATOM	2061	OH2	TIP	1584	18.933	6.009	52.002	1.00	45.27
ATOM	2062	OH2	TIP	1585	-1.653	20.171	69.665	1.00	37.15
ATOM	2063	OH2	TIP	1586	-2.633	4.655	52.475	1.00	49.05
ATOM	2064	OH2	TIP	1587	36.297	28.180	83.444	1.00	41.56
ATOM	2065	OH2	TIP	1588	-0.851	31.806	55.808	1.00	34.41
ATOM	2066	OH2	TIP	1589	4.002	34.625	70.007	1.00	46.13
ATOM	2067	OH2	TIP	1590	32.711	20.152	84.581	1.00	53.56
ATOM	2068	OH2	TIP	1591	19.998	6.099	87.630	1.00	31.12
ATOM	2069	OH2	TIP	1593	-0.189	3.637	35.682	1.00	54.58
ATOM	2070	OH2	TIP	1594	12.455	12.705	39.358	1.00	55.12
ATOM	2071	OH2	TIP	1596	-2.554	-6.074	47.925	1.00	55.01
ATOM	2072	OH2	TIP	1597	5.017	28.176	75.017	1.00	42.02
ATOM	2073	OH2	TIP	1598	28.617	32.433	80.891	1.00	65.40
ATOM	2074	OH2	TIP	1599	8.680	7.258	78.481	1.00	52.56
ATOM	2075	OH2	TIP	1600	18.188	12.950	87.437	1.00	47.03
ATOM	2076	OH2	TIP	1601	-11.532	19.931	55.756	1.00	48.92
ATOM	2077	OH2	TIP	1602	22.073	14.215	52.571	1.00	49.32
ATOM	2078	OH2	TIP	1603	-3.860	34.262	53.170	1.00	48.97

ATOM	2079	OH2	TIP	1604	1.118	10.847	82.180	1.00	44.11
ATOM	2080	OH2	TIP	1605	19.335	32.031	77.782	1.00	48.61
ATOM	2081	OH2	TIP	1606	19.174	9.955	48.654	1.00	40.42
ATOM	2082	OH2	TIP	1607	23.632	-1.631	71.300	1.00	37.97
ATOM	2083	OH2	TIP	1608	26.622	26.695	85.361	1.00	44.14
ATOM	2084	OH2	TIP	1609	22.586	-1.769	57.526	1.00	48.15
ATOM	2085	OH2	TIP	1610	21.977	5.567	60.712	1.00	37.76
ATOM	2086	OH2	TIP	1611	21.634	2.725	67.903	1.00	41.42
ATOM	2087	OH2	TIP	1612	4.046	4.187	75.513	1.00	55.86
ATOM	2088	OH2	TIP	1614	0.807	25.979	47.960	1.00	38.30
ATOM	2089	OH2	TIP	1615	17.333	37.351	72.160	1.00	55.70
ATOM	2090	OH2	TIP	1616	2.475	15.902	62.566	1.00	38.40
ATOM	2091	OH2	TIP	1618	0.658	14.983	64.592	1.00	60.57
ATOM	2092	OH2	TIP	1619	-6.509	17.844	52.643	1.00	41.17
ATOM	2093	OH2	TIP	1621	27.000	-1.287	80.946	1.00	51.49
ATOM	2094	OH2	TIP	1622	3.271	9.154	86.392	1.00	55.17
ATOM	2095	OH2	TIP	1627	3.433	19.409	44.225	1.00	50.54
ATOM	2096	OH2	TIP	1628	2.390	26.629	72.360	1.00	42.60
ATOM	2097	OH2	TIP	1629	9.893	39.104	69.833	1.00	54.40
ATOM	2098	OH2	TIP	1630	2.709	14.153	43.455	1.00	34.37
ATOM	2099	OH2	TIP	1631	11.049	12.448	88.232	1.00	45.81
ATOM	2100	OH2	TIP	1632	4.576	31.506	72.757	1.00	39.34
ATOM	2101	OH2	TIP	1634	6.784	36.285	71.148	1.00	51.53
ATOM	2102	OH2	TIP	1635	6.667	43.335	56.568	1.00	51.21
ATOM	2103	OH2	TIP	1636	-5.771	9.260	60.442	1.00	44.79
ATOM	2104	OH2	TIP	1638	0.052	33.418	66.937	1.00	47.03
ATOM	2105	OH2	TIP	1641	0.354	1.055	46.133	1.00	54.03
ATOM	2106	OH2	TIP	1642	24.406	30.113	88.300	1.00	48.82
ATOM	2107	OH2	TIP	1643	26.619	20.182	66.495	1.00	38.01
ATOM	2108	OH2	TIP	1644	17.492	7.024	42.815	1.00	65.02
ATOM	2109	OH2	TIP	1645	25.942	26.481	82.676	1.00	49.52
ATOM	2110	OH2	TIP	1646	20.601	16.199	68.672	1.00	37.35
ATOM	2111	OH2	TIP	1649	27.616	9.156	63.460	1.00	37.92
ATOM	2112	OH2	TIP	1650	0.428	-3.038	44.190	1.00	54.50
ATOM	2113	OH2	TIP	1652	-7.028	20.462	59.299	1.00	33.58
ATOM	2114	OH2	TIP	1653	-2.848	32.314	67.354	1.00	49.02

ATOM	2115	OH2	TIP	1654	-0.686	17.762	66.362	1.00	46.03
ATOM	2116	OH2	TIP	1655	19.583	17.275	60.162	1.00	41.00
ATOM	2117	OH2	TIP	1656	13.719	36.618	75.139	1.00	51.89
ATOM	2118	OH2	TIP	1657	9.386	-0.422	71.399	1.00	43.15
ATOM	2119	OH2	TIP	1659	23.690	28.880	79.578	1.00	42.62
ATOM	2120	OH2	TIP	1660	22.069	3.800	58.682	1.00	46.06
ATOM	2121	OH2	TIP	1661	20.671	13.353	58.841	1.00	57.05
ATOM	2122	OH2	TIP	1662	27.473	10.135	82.332	1.00	47.43
ATOM	2123	OH2	TIP	1664	9.564	26.542	84.601	1.00	44.55
ATOM	2124	OH2	TIP	1666	29.122	9.606	65.764	1.00	45.20
ATOM	2125	OH2	TIP	1668	13.135	20.507	41.865	1.00	59.09
ATOM	2126	OH2	TIP	1669	22.639	11.672	58.999	1.00	54.98
ATOM	2127	OH2	TIP	1670	-1.845	6.027	76.197	1.00	48.89
ATOM	2128	OH2	TIP	1672	4.883	25.252	42.734	1.00	51.13
ATOM	2129	OH2	TIP	1675	1.329	39.322	66.763	1.00	68.30
ATOM	2130	OH2	TIP	1676	12.783	29.313	87.079	1.00	54.62
ATOM	2131	OH2	TIP	1679	25.035	18.339	57.364	1.00	54.53
ATOM	2132	OH2	TIP	1682	29.392	-1.856	57.721	1.00	37.30
ATOM	2133	OH2	TIP	1683	28.780	9.970	58.622	1.00	54.22
ATOM	2134	OH2	TIP	1685	4.741	39.274	62.499	1.00	46.58
ATOM	2135	OH2	TIP	1686	-3.084	6.977	49.478	1.00	57.17
ATOM	2136	OH2	TIP	1687	26.519	30.868	83.197	1.00	64.53
ATOM	2137	OH2	TIP	1688	-2.784	37.278	67.289	1.00	59.53
ATOM	2138	OH2	TIP	1689	18.691	10.604	88.296	1.00	52.44
ATOM	2139	OH2	TIP	1690	27.919	6.703	82.226	1.00	44.84
ATOM	2140	OH2	TIP	1691	-4.338	11.103	48.033	1.00	55.91
ATOM	2141	OH2	TIP	1692	-7.853	9.429	46.864	1.00	63.74
ATOM	2142	OH2	TIP	1693	10.901	-1.686	67.477	1.00	41.21
ATOM	2143	OH2	TIP	1694	-2.114	6.315	55.259	1.00	56.21
ATOM	2144	OH2	TIP	1695	17.482	15.932	44.391	1.00	41.18
ATOM	2145	OH2	TIP	1696	-12.326	38.088	61.786	1.00	53.30
ATOM	2146	OH2	TIP	1697	-2.176	40.471	68.230	1.00	68.88
ATOM	2147	OH2	TIP	1700	6.514	-1.974	53.366	1.00	51.67
ATOM	2148	OH2	TIP	1701	21.800	10.610	55.773	1.00	60.93
ATOM	2149	OH2	TIP	1702	3.975	27.046	41.446	1.00	44.88
ATOM	2150	OH2	TIP	1703	26.678	-3.660	64.081	1.00	62.42

ATOM 2151 OH2 TIP 1704 2.958 12.027 86.133 1.00 53.52
ATOM 2152 OH2 TIP 1705 4.264 22.050 63.018 1.00 16.96
ATOM 2153 OH2 TIP 1706 22.999 26.329 63.006 1.00 32.17
ATOM 2154 OH2 TIP 1707 5.614 2.688 68.201 1.00 42.08
ATOM 2155 OH2 TIP 1708 -2.967 17.730 54.394 1.00 38.89
ATOM 2156 OH2 TIP 1709 25.853 10.594 62.118 1.00 43.50
ATOM 2157 OH2 TIP 1711 13.060 12.966 86.563 1.00 41.22
ATOM 2158 OH2 TIP 1712 19.784 15.472 45.489 1.00 58.17
ATOM 2159 OH2 TIP 1713 10.567 14.806 42.991 1.00 43.48
ATOM 2160 OH2 TIP 1714 24.079 30.190 83.477 1.00 47.61
ATOM 2161 OH2 TIP 1715 23.927 21.975 63.464 1.00 44.77
ATOM 2162 OH2 TIP 1716 15.801 20.193 58.769 1.00 34.32
ATOM 2163 OH2 TIP 1717 23.867 27.717 72.712 1.00 40.47
ATOM 2164 OH2 TIP 1718 24.567 27.201 69.884 1.00 45.97
ATOM 2165 OH2 TIP 1719 32.141 -1.375 73.278 1.00 62.31
ATOM 2166 OH2 TIP 1720 19.799 24.122 57.454 1.00 35.07
ATOM 2167 OH2 TIP 1721 18.297 23.286 53.598 1.00 43.88
ATOM 2168 OH2 TIP 1722 8.617 1.105 73.470 1.00 48.55
ATOM 2169 OH2 TIP 1723 28.598 25.728 64.296 1.00 46.24
ATOM 2170 OH2 TIP 1725 19.225 33.547 73.276 1.00 44.07
ATOM 2171 OH2 TIP 1726 1.762 4.546 47.584 1.00 50.27
ATOM 2172 OH2 TIP 1727 10.895 28.774 83.657 1.00 54.87
ATOM 2173 OH2 TIP 1728 9.989 36.628 73.713 1.00 46.56
ATOM 2174 OH2 TIP 1729 -1.331 8.332 70.133 1.00 46.76
ATOM 2175 OH2 TIP 1730 24.262 12.802 55.386 1.00 59.24
ATOM 2176 OH2 TIP 1731 28.623 25.788 86.798 1.00 51.87
ATOM 2177 OH2 TIP 1732 -0.501 4.843 68.521 1.00 47.96
ATOM 2178 OH2 TIP 1736 18.422 4.635 54.793 1.00 51.00
ATOM 2179 OH2 TIP 1737 -5.388 27.319 50.727 1.00 46.53
ATOM 2180 OH2 TIP 1738 -2.286 20.842 72.915 1.00 45.95
ATOM 2181 OH2 TIP 1739 0.996 4.268 39.511 1.00 52.67
ATOM 2182 OH2 TIP 1740 -10.886 28.616 64.116 1.00 45.22
ATOM 2183 OH2 TIP 1741 20.353 -4.883 70.512 1.00 61.31
ATOM 2184 OH2 TIP 1742 22.491 16.164 60.365 1.00 58.19
ATOM 2185 OH2 TIP 3001 15.272 21.419 87.789 1.00 27.44
ATOM 2186 OH2 TIP 3002 13.055 32.876 52.925 1.00 53.35

ATOM 2187 OH2 TIP 3006 16.014 18.841 64.083 1.00 56.45
ATOM 2188 OH2 TIP 3008 16.802 30.100 54.388 1.00 48.87
ATOM 2189 OH2 TIP 3009 13.673 27.099 82.740 1.00 32.07
ATOM 2190 OH2 TIP 3010 30.041 24.325 84.969 1.00 41.40
ATOM 2191 OH2 TIP 3007 -2.102 35.612 60.958 1.00 52.05
ATOM 2192 OH2 TIP 3011 7.242 14.501 40.017 1.00 51.46
ATOM 2193 OH2 TIP 3012 1.031 36.834 60.593 1.00 49.05
ATOM 2194 OH2 TIP 3013 0.026 24.244 72.355 1.00 42.35
ATOM 2195 OH2 TIP 3015 -7.871 31.986 57.037 1.00 46.09
ATOM 2196 OH2 TIP 3019 8.655 -3.490 62.423 1.00 44.56
ATOM 2197 OH2 TIP 3020 -0.191 30.553 51.677 1.00 54.31
ATOM 2198 OH2 TIP 3023 3.107 37.905 57.599 1.00 48.07
ATOM 2199 OH2 TIP 3024 26.217 6.182 84.277 1.00 47.75
ATOM 2200 OH2 TIP 3025 2.594 16.520 65.838 1.00 40.67
ATOM 2201 C1 EPH 4000 23.874 12.843 85.264 1.00 42.79
ATOM 2202 C2 EPH 4000 23.099 13.772 86.129 1.00 44.39
ATOM 2203 C4 EPH 4000 24.923 13.000 83.062 1.00 45.55
ATOM 2204 O2 EPH 4000 24.221 13.543 84.059 1.00 44.96
ATOM 2205 O4 EPH 4000 25.350 11.876 83.028 1.00 47.53
ATOM 2206 C18 EPH 4000 25.126 14.045 81.931 1.00 47.05
ATOM 2207 C19 EPH 4000 24.674 13.569 80.547 1.00 46.98
ATOM 2208 C20 EPH 4000 23.168 13.412 80.473 1.00 49.00
ATOM 2209 C21 EPH 4000 22.772 12.939 79.111 1.00 51.06
ATOM 2210 C22 EPH 4000 21.365 12.327 79.073 1.00 52.88
ATOM 2211 C23 EPH 4000 20.291 13.230 78.423 1.00 54.24
ATOM 2212 C24 EPH 4000 20.651 13.777 77.022 1.00 55.08
ATOM 2213 C25 EPH 4000 19.987 15.129 76.704 1.00 56.13
ATOM 2214 C26 EPH 4000 20.807 16.375 77.147 1.00 56.19
ATOM 2215 C27 EPH 4000 19.981 17.687 77.287 1.00 56.74
ATOM 2216 C28 EPH 4000 19.188 18.077 76.015 1.00 56.93
ATOM 2217 C29 EPH 4000 20.055 18.393 74.792 1.00 57.07
ATOM 2218 C30 EPH 4000 19.294 18.387 73.442 1.00 58.24
ATOM 2219 C31 EPH 4000 19.391 17.124 72.550 1.00 58.70
ATOM 2220 C32 EPH 4000 18.019 16.479 72.198 1.00 59.07
ATOM 2221 C33 EPH 4000 16.762 17.158 72.768 1.00 59.61
ATOM 2222 C34 EPH 4000 15.463 16.541 72.231 1.00 60.17

ATOM	2223	C37	EPH	4000	22.780	13.059	87.421	1.00	47.03	
ATOM	2224	O5	EPH	4000	22.047	13.939	88.273	1.00	53.23	
ATOM	2225	P1	EPH	4000	21.699	13.222	89.578	1.00	56.71	
ATOM	2226	O6	EPH	4000	20.350	13.536	89.939	1.00	58.07	
ATOM	2227	O7	EPH	4000	22.579	12.360	90.311	1.00	56.72	
ATOM	2228	O8	EPH	4000	22.167	14.340	90.336	1.00	55.93	
ATOM	2229	C3	EPH	4000	21.561	15.394	85.253	1.00	42.20	
ATOM	2230	O1	EPH	4000	21.886	14.117	85.454	1.00	40.69	
ATOM	2231	O3	EPH	4000	22.221	16.347	85.571	1.00	40.97	
ATOM	2232	C5	EPH	4000	20.215	15.530	84.546	1.00	40.77	
ATOM	2233	C6	EPH	4000	20.313	15.776	83.050	1.00	42.19	
ATOM	2234	C7	EPH	4000	18.924	15.916	82.453	1.00	43.05	
ATOM	2235	C8	EPH	4000	18.900	15.944	80.947	1.00	44.57	
ATOM	2236	C9	EPH	4000	17.477	16.101	80.445	1.00	45.49	
ATOM	2237	C10	EPH	4000	17.167	15.209	79.273	1.00	47.18	
ATOM	2238	C11	EPH	4000	16.561	15.987	78.117	1.00	47.85	
ATOM	2239	C12	EPH	4000	15.158	15.514	77.781	1.00	49.75	
ATOM	2240	C13	EPH	4000	15.158	14.254	76.932	1.00	49.27	
ATOM	2241	C14	EPH	4000	14.899	14.563	75.454	1.00	51.41	
ATOM	2242	C15	EPH	4000	14.958	13.341	74.490	1.00	51.93	
ATOM	2243	C16	EPH	4000	16.376	12.870	74.074	1.00	52.39	
ATOM	2244	C17	EPH	4000	16.681	11.465	74.554	1.00	52.37	
ATOM	2245	C35	EPH	4000	17.830	11.518	75.525	1.00	52.96	
ATOM	2246	C36	EPH	4000	17.968	10.168	76.193	1.00	53.00	
ATOM	2247	C38	EPH	4000	22.197	10.885	90.057	1.00	56.75	
ATOM	2248	C39	EPH	4000	23.458	10.026	89.911	1.00	56.42	
ATOM	2249	N1	EPH	4000	24.546	10.825	89.334	1.00	54.45	
ATOM	2250	N	SER	236	17.914	25.370	86.674	0.50	20.48	AC2
ATOM	2251	CA	SER	236	18.176	23.976	86.323	0.50	19.91	AC2
ATOM	2252	CB	SER	236	19.157	23.889	85.166	0.50	18.72	AC2
ATOM	2253	OG	SER	236	19.325	22.538	84.787	0.50	17.70	AC2
ATOM	2254	C	SER	236	18.741	23.171	87.483	0.50	21.62	AC2
ATOM	2255	O	SER	236	19.744	23.549	88.075	0.50	20.94	AC2
ATOM	2256	N	SER	247	25.235	21.608	79.357	0.50	19.68	AC2
ATOM	2257	CA	SER	247	25.203	22.865	78.619	0.50	20.48	AC2
ATOM	2258	CB	SER	247	26.051	23.917	79.337	0.50	19.95	AC2

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ATOM  2259  OG  SER  247      26.032  25.152  78.637  0.50 20.60      AC2
ATOM  2260  C   SER  247      25.725  22.638  77.203  0.50 20.84      AC2
ATOM  2261  O   SER  247      25.203  23.202  76.238  0.50 21.05      AC2
ATOM  2262  N   SER  271       7.551  30.448  53.176  0.50 29.97      AC2
ATOM  2263  CA  SER  271       7.680  31.880  53.442  0.50 31.61      AC2
ATOM  2264  CB  SER  271       8.888  32.443  52.695  0.50 32.22      AC2
ATOM  2265  OG  SER  271       8.666  32.395  51.295  0.50 32.71      AC2
ATOM  2266  C   SER  271       6.432  32.648  53.010  0.50 32.99      AC2
ATOM  2267  O   SER  271       6.229  33.796  53.408  0.50 34.05      AC2
ATOM  2268  N   PRO  319      18.143  -4.099  74.681  0.50 41.20      AC2
ATOM  2269  CD  PRO  319      18.070  -4.311  76.139  0.50 40.63      AC2
ATOM  2270  CA  PRO  319      18.053  -2.673  74.356  0.50 38.50      AC2
ATOM  2271  CB  PRO  319      17.702  -2.038  75.699  0.50 39.26      AC2
ATOM  2272  CG  PRO  319      18.406  -2.938  76.680  0.50 39.94      AC2
ATOM  2273  C   PRO  319      19.321  -2.077  73.756  0.50 35.96      AC2
ATOM  2274  O   PRO  319      20.410  -2.230  74.313  0.50 35.87      AC2
ATOM  2275  N   GLN  343      13.913   5.584  80.085  0.50 18.73      AC2
ATOM  2276  CA  GLN  343      12.714   5.137  79.387  0.50 19.83      AC2
ATOM  2277  CB  GLN  343      11.463   5.365  80.243  0.50 21.34      AC2
ATOM  2278  CG  GLN  343      10.903   4.078  80.837  0.50 26.09      AC2
ATOM  2279  CD  GLN  343       9.539   4.244  81.488  0.50 27.02      AC2
ATOM  2280  OE1 GLN  343       9.412   4.823  82.562  0.50 29.15      AC2
ATOM  2281  NE2 GLN  343       8.508   3.730  80.829  0.50 29.67      AC2
ATOM  2282  C   GLN  343      12.545   5.813  78.025  0.50 19.53      AC2
ATOM  2283  O   GLN  343      12.317   5.141  77.022  0.50 19.10      AC2
ATOM  2284  N   SER  353      14.027   4.461  65.783  0.50 19.97      AC2
ATOM  2285  CA  SER  353      15.191   3.950  65.107  0.50 20.43      AC2
ATOM  2286  CB  SER  353      16.391   4.058  66.033  0.50 20.57      AC2
ATOM  2287  OG  SER  353      17.540   4.234  65.262  0.50 19.64      AC2
ATOM  2288  C   SER  353      15.054   2.524  64.574  0.50 21.08      AC2
ATOM  2289  O   SER  353      15.234   2.291  63.378  0.50 21.51      AC2
ATOM  2290  N   ARG  392       0.696  20.186  53.122  0.50 19.50      AC2
ATOM  2291  CA  ARG  392       0.935  18.822  53.549  0.50 19.96      AC2
ATOM  2292  CB  ARG  392       0.325  18.551  54.925  0.50 19.99      AC2
ATOM  2293  CG  ARG  392       0.603  17.129  55.384  0.50 19.08      AC2
ATOM  2294  CD  ARG  392       0.140  16.884  56.805  0.50 19.85      AC2
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ATOM   2295  NE  ARG   392      -1.315  16.885  56.925  0.50 19.23      AC2
ATOM   2296  CZ  ARG   392      -1.962  16.577  58.046  0.50 21.63      AC2
ATOM   2297  NH1 ARG   392      -1.283  16.242  59.138  0.50 19.92      AC2
ATOM   2298  NH2 ARG   392      -3.289  16.611  58.086  0.50 22.19      AC2
ATOM   2299  C   ARG   392       0.338  17.878  52.501  0.50 19.95      AC2
ATOM   2300  O   ARG   392       0.940  16.867  52.149  0.50 20.64      AC2
ATOM   2301  N   SER   431       9.466  14.172  75.955  0.50 16.96      AC2
ATOM   2302  CA  SER   431      10.735  14.900  76.047  0.50 17.25      AC2
ATOM   2303  CB  SER   431      11.346  15.109  74.659  0.50 17.09      AC2
ATOM   2304  OG  SER   431      10.765  16.211  73.998  0.50 16.93      AC2
ATOM   2305  C   SER   431      10.466  16.249  76.719  0.50 17.71      AC2
ATOM   2306  O   SER   431      11.267  16.716  77.521  0.50 17.14      AC2
END
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Table 2:

bdrxra	----FNEEMPVEKILDAELAV--------------EPKTEAYME----------------
murxra	----ANEDMPVEKILEAELAV--------------EPKTETYVE----------------
rnrxra	----ANEDMPVEKILEAELAV--------------EPKTETYVE----------------
horxra	----ANEDMPVERILEAELAV--------------EPKTETYVE----------------
xlrxra	----ANEDMPVEKILEAEHAV--------------EPKTETYTE----------------
surxrb	--
aeuspa	-----VRDVTIERIHEAEQLS-----E--------QKSGDNAIPYLR-------------
dmusp	MTNSVSRDFSIERIIEAEQRA-----E--------TQCGDRALTFLR-------------
horxrb	----APEEMPVDRILEAELAV--------------EQKSDQGVEGP--------------
murxrb	----APEEMPVDRILEAELAV--------------EQKSDQGVEGP--------------
rnrxrb	----APEEMPVDRILEAELAV--------------EQKSDQGVEGP--------------
xlrxrbb	----INEEMPVEKILEAELAV--------------EQKSDQSLE----------------
xlrxrba	----INEEMPVEKILEAELAV--------------EQKSDQSLE----------------
murxrg	----SHEDMPVERILEAELAV--------------EPKTESYGD----------------
horxrg	----GHEDMPVERILEAELAV--------------EPKTESYGD----------------
garxrg	----GSEDMPVERILEAELAV--------------EPKTEAYSD----------------
xlrxrg	----TSEEMPVERILEAELAV--------------DPKIEAFGD----------------
pmrxr	----PNDDMPVDKILEAELIS--------------DPKVEQVVP----------------
lmrxr	----LHTDMPVERILEAEKRV--------------E------------------------
smrxr	---TDLPNLTLRCLLSAELSM--------------DPKLAVSERG---------------
amusp	----LHSDMPIERILEAEKRV--------------ECKMEQQGN----------------
tmusp	----MQAEMPLDRIIEAEKRI--------------ECTPAGGSG----------------
aarxr	---GAPPEMPLERILEAELRV--------------ESQTGTLSES---------------
aarxr2	--P-GSPDMPLERILEAEMRV--------------EQPAPSVLAQ---------------
uprxr	----AISDMPIASIREAELSV--------------DPIDEQPLDQGVRLQVPLAPPDSEK
cfusp	--VQVSDELSIERLTEMESLV------ADPSEE------FQFLR----------------
msusp	-----VQELSIERLLEIESLV------ADPPEE------FQFLR----------------
bmusp	-----VQELSIERLLELEALV------ADSAEE------LQILR----------------
ctusp	--NGPGRDITVERLMEADQMS------EARCGDKS----IQYLR---------V------
uspx	---AAAQELSIERLLEMESLVAAAAEE------------FQFLR----------------
rxrmin	-ASSANEDMPVEKILEAELAV--------------EPKTETYVE----------------

bdrxra	---------SSM---SNSTNDPVTNICQAADKQLFTLVEWAKRIPHFSDL---PLDDQVI
murxra	---------ANMGLNPSSPNDPVTNICQAADKQLFTLVEWAKRIPHFSEL---PLDDQVI
rnrxra	---------ANMGLNPSSPNDPVTNICQAADKQLFTLVEWAKRIPHFSEL---PLDDQVI
horxra	---------ANMGLNPSSPNDPVTNICQAADKQLFTLVEWAKRIPHFSEL---PLDDQVI
xlrxra	---------ANMGLAPNSPSDPVTNICQAADKQLFTLVEWAKRIPHFSDV---PLDDQVI
surxrb	-------------GSGSSPNDPVTNICQAADKQLFTLVEWAKRIPHFSSL---PLDDQVI
aeuspa	--------VGSNSMIPPEYKGAVSHLCQMVNKQIYQLIDFARRVPHFINL---PRDDQVM
dmusp	--------VGPYSTVQPDYKGAVSALCQVVNKQLFQMVEYARMMPHFAQV---PLDDQVI
horxrb	---------GATGGGGSSPNDPVTNICQAADKQLFTLVEWAKRIPHFSSL---PLDDQVI
murxrb	---------GATGGGGSSPNDPVTNICQAADKQLFTLVEWAKRIPHFSSL---PLDDQVI
rnrxrb	---------GATGGGGSSPNDPVTNICQAADKQLFTLVEWAKRIPHFSSL---PLDDQVI
xlrxrbb	--------------GGGSPSDPVTNICQAADKQLFTLVEWAKRIPHFSEL---ALDDQVI
xlrxrba	--------------GGGSPSDPVTNICQDADKQLFTLVEWAKRIPHFSELPELPLDDQVI
murxrg	------------MNVENSTNDPVTNICHAADKQLFTLVEWAKRIPHFSDL---TLEDQVI
horxrg	------------MNMENSTNDPVTNICHAADKQLFTLVEWAKRIPHFSDL---TLEDQVI
garxrg	------------VNTESSTNDPVTNICHAADKQLFTLVEWAKRIPHFSDL---TLEDQVI
xlrxrg	------------AGLPNSTNDPVTNICHAADKQLFTLVEWAKRIPYFSDL---PLEDQVI
pmrxr	-------------FEQVNENDPVSNICKAADRQLVTLVEWAKRIPHFSSL---PLEDQVI
lmrxr	--------------------------CKAENQVEYELVEWAKHIPHFTSL---PLEDQVL
smrxr	-----EAIYEDIPGDDDTGLHPLTIICQSIEQQLPRIVNWARQLPVFSSVY-LSFDDQFC
amusp	------------------YENAVSHICNATNKQLFQLVAWAKHIPHFTSL---PLEDQVL
tmusp	--------------GVGEQHDGVNNICQATNKQLFQLVQWAKLIPHFTSL---PMSDQVL
aarxr	----------------AQQQDPVSSICQAADRQLHQLVQWAKHIPHFEEL---PLEDRMV
aarxr2	--------------TAASGRDPVNSMCQAAP-PLHELVQWARRIPHFEEL---PIEDRTA
uprxr	CSFTLPFHPVSEVSCANPLQDVVSNICQAADRHLVQLVEWAKHIPHFTDL---PIEDQVV

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cfusp      --------VGPDSNVPPRYRAPVSSLCQIGNKQIAALVVWARDIPHFGQL---ELDDQVV
msusp      --------VGPESGVPAKYRAPVSSLCQIGNKQIAALVVWARDIPHFGQL---ELEDQIL
bmusp      --------VGPESGVPAKYRAPVSSLCQIGNKQIAALIVWARDIPHFGQL---EIDDQIL
ctusp      --------AASNTMIPPEYRAPVSAICAMVNKQVFQHMDFCRRLPHFTKL---PLNDQMY
uspx       --------VGPDSNVPPKFRAPVSSLCQIGNKQIAALVVWARDIPHFSQL---EMEDQIL
rxrmin     ---------ANMGLNPSSPNDPVTNICQAADKQLFTLVEWAKRIPHFSEL---PLDDQVI
                                     *          : :.: :* * .:     .*:

bdrxra     LLRAGWNELLIASFSHRSVTVKDG--------------------------ILLATGLHVH
murxra     LLRAGWNELLIASFSHRSIAVKDG--------------------------ILLATGLHVH
rnrxra     LLRAGWNELLIASFSHRSIAVKDG--------------------------ILLATGLHVH
horxra     LLRAGWNELLIASFSHRSIAVKDG--------------------------ILLATGLHVH
xlrxra     LLRAGWNELLIASFSHRSIAVKDG--------------------------ILLATGLHVH
surxrb     LLRAGWNELLIASFSHRSIDVRDG--------------------------ILLATGLHVH
aeuspa     LLRCGWNEMLIAAVAWRSMEYIETER----------SSDGSRITVRQPQLMCLGPNFTLH
dmusp      LLKAAWIELLIANVAWCSIVSLDDGGGGGGGGLGHDGSFERRSPGLQPQQLFLNQSFSYH
horxrb     LLRAGWNELLIASFSHRSIDVRDG--------------------------ILLATGLHVH
murxrb     LLRAGWNELLIASFSHRSIDVRDG--------------------------ILLATGLHVH
rnrxrb     LLRAGWNELLIASFSHRSIDVRDG--------------------------ILLATGLHVH
xlrxrbb    LLRAGWNELLIASFSHRSISVKDG--------------------------ILLATGLHVH
xlrxrba    LLRAGWNELLIASFSHRSISEKDG--------------------------ILLATGLHVH
murxrg     LLRAGWNELLIASFSHRSVSVQDG--------------------------ILLATGLHVH
horxrg     LLRAGWNELLIASFSHRSVSVQDG--------------------------ILLATGLHVH
garxrg     LLRAGWNELLIASFSHRSVSVQDG--------------------------ILLATGLHVH
xlrxrg     LLRAGWNELLIASFSHRSVSVQDG--------------------------ILLATGLHVH
pmrxr      LLRAGWNELLIASFSHRSIDVKDS--------------------------ILLASGLHVH
lmrxr      LLRAGWNELLIAAFSHRSVDVKDG--------------------------IVLATGLTVH
smrxr      LIKAAWPELVLISSAYHSTVIRDG--------------------------LLLSIGRHLG
amusp      LLRAGWNELLIASFSHRSIDVKDG--------------------------IVLATGITVH
tmusp      LLRAGWNELLIAAFSHRSIQAQDA--------------------------IVLATGLTVN
aarxr      LLKAGWNELLIAAFSHRSVDVRDG--------------------------IVLATGLVVQ
aarxr2     LLKAGWNELLIAAFSHRSVAVRDG--------------------------IVLATGLVVQ
uprxr      LLKAGWNELLIASFSHRSMGVEDG--------------------------IVLATGLVIH
cfusp      LIKASWNELLLFAIAWRSMEYLEDER----------ENGDGTRSTTQPQLMCLMPGMTLH
msusp      LIKNSWNELLLFAIAWRSMEYLTDER----------ENVD-SRSTAPPQLMCLMPGMTLH
bmusp      LIKGSWNELLLFAIAWRSMEFLNDER----------ENVD-SRNTAPPQLICLMPGMTLH
ctusp      LLKQSLNELLILNIAYMSIQYVEPDRRNADG---------SLERRQISQQMCLSRNYTLG
uspx       LIKGSWNELLLFAIAWRSMEFLTAAAAS------------------PPQLMCLMPGMTLH
rxrmin     LLRAGWNELLIASFSHRSIAVK--------------------------DGILLATGLHVH
           *:: .  *:::   :  *                                : *  .

bdrxra     RSSAHSAGVGSIFDRVLTELVSKMRDMQMDKTELGCLRAIVLFNPDAKGLSNPSEVEALR
murxra     RNSAHSAGVGAIFDRVLTELVSKMRDMQMDKTELGCLRAIVLFNPDSKGLSNPAEVEALR
rnrxra     RNSAHSAGVGAIFDRVLTELVSKMRDMQMDKTELGCLRAIVLFNPDSKGLSNPAEVEALR
horxra     RNSAHSAGVGAIFDRVLTELVSKMRDMQMDKTELGCLRAIVLFNPDSKGLSNPAEVEALR
xlrxra     RNSAHSAGVGAIFDRVLTELVSKMRDMQMDKTELGCLRAIVLFNPDSKGLSNPLEVEALR
surxrb     RNSAHSAGVGAIFDRVLTELVSKMRDMRMDKTELGCLRAIILFNPDAKGLSNPSEVEVLR
aeuspa     RNSAQQAGVDTLFDRILCELGIKMKRLDVTRAELGVLKAIILFNPDIRGLKCQKEIDGMR
dmusp      RNSAIKAGVSAIFDRILSELSVKMKRLNLDRRELSCLKAIILYNPDIRGIKSRAEIEMCR
horxrb     RNSAHSAGVGAIFDRVLTELVSKMRDMRMDKTELGCLRAIILFNPDAKGLSNPGEVEILR
murxrb     RNSAHSAGVGAIFDRVLTELVSKMRDMRMDKTELGCLRAIILFNPDAKGLSNPGEVEILR
rnrxrb     RNSAHSAGVGAIFDRVLTELVSKMRDMRMDKTELGCLRAIILFNPDAKGLSNPGEVEILR
xlrxrbb    RNSAHSAGVGAIFDRVLTELVSKMRDMRMDKTELGCLRAIILFNPDAKGLSNPGDVEVLR
xlrxrba    RNSAHSAGVGAIFERVLTELVSKMRDMRMDKTELGCLRAIILFNPDAKGLSNPGDVEVLR
murxrg     RSSAHSRGVGSIFDRVLTELVSKMKDMQMDKSELGCLRAIVLFNPDAKGLSNPSEVETLR
horxrg     RSSAHSAGVGSIFDRVLTELVSKMKDMQMDKSELGCLRAIVLFNPDAKGLSNPSEVETLR
garxrg     RSSAHSAGVGSIFDRVLTELVSKMKDMQMDKSELGCLRAIVLFNPDAKGLSSPSEVESLR
xlrxrg     RSSAHNAGVGSIFDRVLTELVSKMKDMDMDKSELGCLRAIVLFNPDAKGLSNAAEVEALR
pmrxr      RHSAHQAGVGPIFDRVLTELVSKMRDMMMDKTELGCLRAIVLFNPDVKNLSDSAHIESLR
lmrxr      RNSAHQAGVGTIFDRVLTELVAKMREMKMDKTELGCLRSVILFNPEVRGLKSAQEVELLR
smrxr      REVAKSHGLGPLVDRILHELVARFRDLSLQRTELALLRAIILFNPDANGLSSRHRVEAVR
amusp      RNSAQQAGVGTIFDRVLSELVSKMREMKMDRTELGCLRSIILFNPEVRGLKSIQEVTLLR
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tmusp       KTSAHAVGVGNIYDRVLSELVNKMKEMKMDKTELGCLRAIILYNPTCRGIKSVQEVEMLR
aarxr       RHSAHGAGVGAIFDRVLTELVAKMREMKMDRTELGCLLAVVLFNPEAKGLRTCPSGGPEG
aarxr2      RHSAHGAGVGDIFDRVLAELVAKMRDMKMDKTELGCLRAVVLFNPDAKGLRNATRVEALR
uprxr       RSSAHQAGVGAIFDRVLSELVAKMKEMKIDKTELGCLRSIVLFNPDAKGLNCVNDVEILR
cfusp       RNSAQQAGVGAIFDRVLSELSLKMRTLRMDQAEYVALKAIVLLNPDVKGLKNRQEVDVLR
msusp       RNSALQAGVGQIFDRVLSELSLKMRTLRMDQAEYVALKAIILLNPDVKGLKNKPEVVVLR
bmusp       RNSALQAGVGQIFDRVLSELSLKMRSLRMDQAECVALKAIILLNPDVKGLKNKQEVDVLR
ctusp       RNMAVQAGVVQIFDRILSELSVKMKRLDLDATELCLLKSIVVFNPDVRTLDDRKSIDLLR
uspx        RNSALQAGVGQIFDRVLSELSLKMRTLRVDQAEYVALKAIILLNPDVKGLKNRQEVEVLR
rxrmin      RNSAHSAGVGAIFDRVLTELVSKMRDMQMDKTELGCLRAIVLFNPDSKGLSNPAEVEALR
            :   *    *:   :  :*:* **   :::  :  :    *    *  ::::  **   .  :

bdrxra      EKVYASLEGYTKHNYPDQPGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
murxra      EKVYASLEAYCKHKYPEQPGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
rnrxra      EKVYASLEAYCKHKYPEQPGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
horxra      EKVYASLEAYCKHKYPEQPGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
xlrxra      EKVYASLEAYCKQKYPEQPGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
surxrb      EKVYASLETYCKQKYPEQQGRFAKLLLRLPALRSIGLKCLEHLFFFKLI-----------
aeuspa      EKIYACLDEHCKQQHPSEDGRFAQLLLRLPALRSISLKCLDHLNFIRLLSDKHLDSFIVE
dmusp       EKVYACLDEHCRLEHPGDDGRFAQLLLRLPALRSISLKCQDHLFLFRITSDRPLEELFLE
horxrb      EKVYASLETYCKQKYPEQQGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
murxrb      EKVYASLETYCKQKYPEQQGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
rnrxrb      EKVYASLETYCKQKYPEQQGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
xlrxrbb     EKVYASLESYCKQKYPDQQGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
xlrxrba     EKVYACLESYCKQKYPDQQGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
murxrg      EKVYATLEAYTKQKYPEQPGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDSFLME
horxrg      EKVYATLEAYTKQKYPEQPGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
garxrg      EKVYATLEAYTKQKYPEQPGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
xlrxrg      EKVYATLESYTKQKYPDQPGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
pmrxr       EKVYASLEAYCRSKYPDQPGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDKFLMN
lmrxr       EKVYAALEEYTRTTHPDEPGRFAKLLLRLPSLRSIGLKCLEHLFFFRLIGDVPIDTFLME
smrxr       EQLYSALHSYCTTNQPQDTSRFTKLLLRLPPLRSIASKCLEHLVFVKLAAEDPTSCRLIN
amusp       EKIYGALEGYCRVAWPDDAGRFAKLLLRLPAIRSIGLKCLEYLFFFKMIGDVPIDDFLVE
tmusp       EKIYGVLEEYTRTTHPNEPGRFAKLLLRLPALRSIGLKCSEHLFFFKLIGDVPIDTFLME
aarxr       ESV-SALEEHCRQQYPDQPGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDNFLLS
aarxr2      EKVYAALEEHCRRHHPDQPGRFGKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDSFLLN
uprxr       EKVYAALEEYTRTTYPDEPGRFAKLLLRLPALRSIGLKCLEYLFLFKLIGDTPLDSYLMK
cfusp       EKMFSCLDDYCRRSRSNEEGRFASLLLRLPALRSISLKSFEHLYFFHLVAEGSISGYIRE
msusp       EKMFSCLDEYVRRSRCAEEGRFAALLLRLPALRSISLKCFEHLYFFHLVADTSIASYIHD
bmusp       EKMFLCLDEYCRRSRGGEEGRFAALLLRLPALRSISLKSFEHLYLFHLVAEGSVSSYIRD
ctusp       SRIYASLDEYCRQKHPNEDGRFAQLLLRLPALRSISLKCLDHLFYFQLIDDKNVENSVIE
uspx        EKMFLCLDEYCRRSRSSEEGRFAALLLRLPALRSISLKSFEHLFFFHLVADTSIAGYIRD
rxrmin      EKVYASLEAYCKHKYPEQPGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
            .  :    *.  :          :  .**   ******.:***.  *.  ::*   .::

bdrxra      MLEAPHQIT
murxra      MLEAPHQAT
rnrxra      MLEAPHQTT
horxra      MLEAPHQMT
xlrxra      MLEAPHQMT
surxrb      ---------
aeuspa      MLDMPI---
dmusp       QLEAPPPPG
horxrb      MLEAPHQLA
murxrb      MLEAPHQLA
rnrxrb      MLEAPHQLA
xlrxrbb     MLEAPHQLS
xlrxrba     MLEAPHQLS
murxrg      MLETPLQIT
horxrg      MLETPLQIT
garxrg      MLETPLQVT
xlrxrg      MLETPHQIS
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pmrxr           MLETTSDFP
lmrxr           MLESPSDS-
smrxr           LVEHGVWPI
amusp           MLESRSDP-
tmusp           MLESPADA-
aarxr           MLEAPSDP-
aarxr2          MLEAPADP-
uprxr           MLVDNPNTS
cfusp           ALRNHAPPI
msusp           ALRNHAPSI
bmusp           ALCNHAPPI
ctusp           EFHKLN---
uspx            ALRNGG---
rxrmin          MLEAP----
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